



## SM358

Glossary for all books

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Numbers in parentheses are page references with B1, B2, B3 denoting Book 1 (*Wave mechanics*), Book 2 (*Quantum mechanics and its interpretation*) and Book 3 (*Quantum mechanics of matter*) respectively.

Italicized words are cross-references to other entries in this Glossary.

Look on the course website for other glossaries relevant to SM358. These include: (a) the *Physics Toolkit*, which is a glossary of background physics terms, (b) an extract of the full glossary for Book 1 only and (c) an extract of the full glossary for Books 1 and 2 only. The last two may be useful as you study each book in turn.

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**A-coefficient** (B3: 216) Another term for the *Einstein A-coefficient*.

**absolute temperature** A temperature measured on the *absolute temperature scale*.

**absolute temperature scale** The *SI* scale of temperature measured in *kelvin* (K). On this scale, the lowest conceivable temperature, *absolute zero*, is 0 K.

**absolute zero** The lowest conceivable temperature for any *system*. It is represented by the value 0 K on the *absolute temperature scale*, and corresponds to a temperature of  $-273.15^{\circ}\text{C}$  on the Celsius temperature scale. In *classical physics*, where temperature is a measure of molecular agitation, absolute zero corresponds to all *particles* being in a *state* of rest with a minimum mutual *potential energy*.

**absorption** (B3: 196) A process in which a *system* absorbs a *photon* of energy  $hf$  and makes a *radiative transition* from an initial *quantum state* of energy  $E_i$  to a final quantum state of energy  $E_f$ , with  $E_f > E_i$ . After the transition, the photon ceases to exist, but the law of *conservation of energy* is respected because  $E_f = E_i + hf$ . The rate of absorption is proportional to the *Einstein B-coefficient*, which can be calculated using the *electric dipole approximation* and *time-dependent perturbation theory*. Compare with *spontaneous emission* and *stimulated emission*.

**abstract vector** A *vector* in a *vector space*, which need not be the same as ordinary three-dimensional space.

**acceptor atom** (B3: 191) A type of impurity *atom* in a *semiconductor* that can accept *electrons* from the

*valence band* of the semiconductor, leaving *holes* in their place. With a sufficient *number density* of acceptor atoms a *p-type semiconductor* can be produced. Acceptor atoms for silicon or germanium include boron, aluminium, gallium and indium in *Group 13* of the *Periodic Table*. Contrast with *donor atom*.

**addition rule for probability** (B1: 228) This mathematical rule states that the *probability* of obtaining one or other of a set of *mutually exclusive outcomes* in a single trial or experiment is the sum of their individual probabilities.

**alkali atoms** (B3: 129) *Atoms* of *elements* (except *hydrogen*) in the first *group* of the *Periodic Table*, namely lithium (Li), sodium (Na), potassium (K), rubidium (Rb), caesium (Cs) and francium (Fr). Alkali atoms have a single *valence electron* in an *s-shell*, with the other *electrons* forming a tightly-bound core around the *nucleus*. They react strongly with *halogen atoms*.

**alpha decay** (B1: 203) A form of *radioactive decay* in which the *nucleus* of an *atom* ejects an energetic *alpha particle*. As a result, the *atomic number*  $Z$  of the emitting nucleus is reduced by two, and its *mass number*  $A$  is reduced by four.

Alpha decay involves the *tunnelling* of alpha particles through a *Coulomb barrier*. See also the *Geiger–Nuttall relation*.

**alpha particle** (B1: 12) A type of composite *particle*, consisting of two *protons* and two *neutrons* bound together. An alpha particle is identical to the *nucleus* of a *helium atom* with *mass number* 4, and is therefore the same as a doubly-ionized helium-4 atom. The term is generally used in the context of alpha-particle emission from certain unstable nuclei in the *radioactive decay* process known as *alpha decay*.  
BOOK 2: Alpha particles are *bosons*.

**amorphous solid** (B3: 169) A solid material that does not have a *crystalline structure*. Glass is an example of an amorphous solid. Silicon, metals and ice can also be prepared in amorphous forms.

**amplitude** (B1: 17, 125) The *magnitude* of the maximum deviation of an *oscillation* or *wave* from equilibrium. For a *sinusoidal* oscillation described by the function  $x(t) = A \cos(\omega t + \phi)$ , the positive constant  $A$  is the amplitude of the oscillation. For a sinusoidal wave described by the function  $u(x, t) = A \cos(kx - \omega t + \phi)$ , the positive constant  $A$  is the amplitude of the wave.

In *quantum physics*, the word ‘amplitude’ is sometimes used as a shorthand for *probability amplitude*; this should not be confused with the amplitude of an oscillation or wave.

**angular frequency** (B1: 10, 17, 126) The rate of change of the *phase* of an *oscillation* or *wave*. The angular frequency  $\omega$  is given by

$$\omega = 2\pi f = \frac{2\pi}{T},$$

where  $f$  is the *frequency* and  $T$  is the *period* of the oscillation or wave. The *SI* unit of angular frequency is the inverse second,  $\text{s}^{-1}$ . (Some authors use  $\text{rad s}^{-1}$ , but this clashes with the fact that product of angular frequency and time appears in functions such as  $\sin(\omega t)$  and, in this context,  $\omega t$  must be a pure number to ensure that an expansion of the sine function gives a power series in which different terms have the same units.)

**angular momentum** (B2: 40) A quantity that describes a *state* of rotational motion. In *classical physics*, the angular momentum of *particle* about an origin  $O$  is defined by the *vector product*

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

where  $\mathbf{r}$  is the displacement of the particle from  $O$  and  $\mathbf{p}$  is the *momentum* of the particle. The *SI* unit of angular momentum is  $\text{kg m}^2 \text{s}^{-1}$ .

A classical rigid body rotating about a fixed axis has a *component* of angular momentum along the axis of *magnitude*

$$L = I\omega,$$

where  $I$  is the *moment of inertia* of the body about the fixed axis of rotation and  $\omega$  is the angular speed of the

body about this axis. If the axis of rotation is an axis of symmetry (or a so-called principal axis), there are no components of angular momentum perpendicular to the axis of rotation, and the magnitude of the angular momentum is  $I\omega$ . (This is the only case of rigid body rotation considered in this course).

In *quantum physics*, the above type of angular momentum, which involves the motion of particles or bodies, is called *orbital angular momentum*. Certain types of particle have an additional angular momentum which would be present even if the particles did not move; this is called *intrinsic angular momentum* or *spin angular momentum*. The *total angular momentum* of any *system* is the *vector* sum of all the orbital and spin angular momentum contributions. Each component of angular momentum is represented by a quantum-mechanical *angular momentum operator*.

**angular momentum operators** (B2: 48)

Quantum-mechanical *operators* representing *components* of *angular momentum*. See *orbital angular momentum operators*, *spin angular momentum operators*. BOOK 3: See also *total angular momentum operators*.

**anharmonic oscillator** (B3: 78) An oscillator for which the *potential energy function* is not proportional to the square of the displacement from the equilibrium position. Contrast with *harmonic oscillator*.

**antibonding orbital** (B3: 157) A *molecular orbital* for which the *energy* is always higher than either of the energies of the *atomic orbitals* from which it is formed. The *energy curve* for an antibonding orbital has no minimum at finite internuclear separations and the *probability density* for *electrons* in the region between the *atoms* is low. Contrast with *bonding orbital*.

**antiparticle** (B3: 109) All *elementary particles* with mass, stable and unstable, have antiparticles. An antiparticle has exactly the same mass as the corresponding particle, but it has the opposite signs for other attributes, such as *electric charge*. When a particle collides with its own antiparticle, the two may annihilate each other completely, producing *electromagnetic radiation* (usually gamma rays).

**antiproton** (B3: 99) The negatively-charged *antiparticle* of the *proton*.

**antisymmetric function** (B2: 110) A function  $f(x_1, x_2)$  is said to be antisymmetric with respect to exchange of the labels 1 and 2 if

$$f(x_2, x_1) = -f(x_1, x_2)$$

More generally, a function of many variables is antisymmetric if it changes sign when any two of its variables are exchanged.

A *singlet spin state* is antisymmetric and the *spatial*

wave function of a pair of electrons in a triplet state is antisymmetric. Contrast with *symmetric function*.

**arbitrary constant** (B1: 218) A constant that appears in the *general solution* of a *differential equation* but does not appear in the differential equation itself. If the *order of a differential equation* is  $n$ , the general solution of the equation contains  $n$  arbitrary constants. The arbitrary constants serve to distinguish one *particular solution* from another.

**Argand diagram** (B1: 212) Another term for the *complex plane*.

**argument** (B1: 213) (i) A term for the *phase* of a *complex number*.

(ii) Another term for an expression within a function; for example, the argument of  $\sin(kx)$  is  $kx$ .

**atom** The smallest electrically-neutral sample of an *element* that retains the fundamental chemical and physical identity of that element. An atom consists of a positively-charged *nucleus* surrounded by a cloud of negatively-charged *electrons*. Most of the mass of an atom is contained in its nucleus, but atomic sizes are generally determined by the distribution of electrons. Atomic radii vary from about  $5 \times 10^{-11}$  m to  $3 \times 10^{-10}$  m.

**atomic levels** (B3: 137) The *energy levels* that an *atomic term* splits into as a result of the *spin-orbit interaction*.

In the *LS-coupling scheme*, an atomic level is characterized by the *quantum numbers*  $L$ ,  $S$  and  $J$  (the *total orbital angular momentum quantum number*, the *total spin quantum number* and the *total angular momentum quantum number*). The *spectroscopic notation* for an atomic level is

$$^{2S+1}L_J,$$

where  $L$  is equal to S, P, D, F, ... for  $L = 0, 1, 2, 3, \dots$ . For given values of  $L$  and  $S$ , the possible values of  $J$  are

$$|L - S|, |L - S| + 1, \dots, |L + S| - 1, |L + S|.$$

Each atomic level corresponds to  $(2J + 1)$  *degenerate quantum states* distinguished by the *total magnetic quantum number*  $M_J$ , which takes the values  $-J, -J + 1, \dots, J - 1, J$ .

**atomic number** (B1: 12) The number of *protons* in the *nucleus* of a particular type of *atom*, and hence the number of *electrons* in the neutral atom. An *element* is identified by its atomic number  $Z$ , which determines its chemical properties. The atomic number is usually denoted by the symbol  $Z$ ; *hydrogen*, *helium* and *lithium* atoms have  $Z = 1, 2$  and  $3$  respectively.

**atomic orbital** (B3: 117) An *eigenfunction* of a single-particle *time-independent Schrödinger*

*equation*, used to model the *quantum state* of an *electron* in an *atom* in the *central-field approximation*.

**atomic terms** (B3: 134) In the *LS-coupling scheme* an *electronic configuration* of an *atom* gives rise to a set of atomic terms, each characterized by a pair of *quantum numbers*,  $L$  and  $S$ , the *total orbital angular momentum quantum number* and the *total spin quantum number*. The *spectroscopic notation* for an atomic term is

$$^{2S+1}L,$$

where  $L$  is equal to S, P, D, F, ... for  $L = 0, 1, 2, 3, \dots$

Residual electron-electron interactions (not included in the *central-field approximation*) cause different atomic terms to have different *energies*. Each atomic term corresponds to  $(2L + 1)(2S + 1)$  *degenerate quantum states* distinguished by the quantum numbers  $M_L$  and  $M_S$ , where  $M_L$  takes the values  $-L, -L + 1, \dots, L - 1, L$  and  $M_S$  takes the values  $-S, -S + 1, \dots, S - 1, S$ .

The *spin-orbit interaction* produces *fine structure*: the atomic term  $^{2S+1}L$  splits into  $2S + 1$  *atomic levels* if  $L \geq S$  (and  $2L + 1$  atomic levels if  $L < S$ ). In spite of the phrase in brackets, the quantity  $2S + 1$  is always called the *multiplicity* of the atomic term.

**attenuation coefficient** (B1: 199) A *real* quantity that determines the rate of exponential decrease of some other quantity with increasing distance. An example is the quantity  $\alpha$  that appears in the expression  $Ce^{-\alpha|x|}$ , which is the form of a *bound state energy eigenfunction* for a *particle* in one of the *classically-forbidden regions* outside a one-dimensional *finite square well*. The SI unit of an attenuation coefficient is  $m^{-1}$ .

**auxiliary equation** (B1: 219) An algebraic equation obtained when a trial solution containing undetermined parameters is substituted into a *differential equation*. The auxiliary equation determines possible values of these parameters.

**average value** (B1: 228) If a quantity  $A$  is measured  $N$  times in a given situation, and the result  $A_i$  is obtained on  $N_i$  occasions, the average value of  $A$  over the set of measurements is defined to be

$$\bar{A} = \frac{1}{N} \sum_{i=1}^N N_i A_i = \sum_{i=1}^N f_i A_i,$$

where the sum is over all the outcomes and  $f_i = N_i/N$  is the *relative frequency* of outcome  $i$ .

The measured average value  $\bar{A}$  is expected to approach the theoretical *expectation value*  $\langle A \rangle$  as the number of measurements becomes very large. Also called the *mean value*.

**azimuthal angle** (B3: 12) An angle of rotation around the  $z$ -axis, denoted by  $\phi$  and measured



in radians. The azimuthal angle lies in the range  $0 \leq \phi \leq 2\pi$  and is equal to 0 or  $2\pi$  along the positive  $x$ -axis. It increases in the sense of the curled fingers of the right hand when the outstretched thumb of the right hand points along the  $z$ -axis (an example of the *right-hand grip rule*). The azimuthal angle is one of the *spherical coordinates*, together with the *polar angle* and the *radial coordinate*.

**azimuthal quantum number** Another term for the *magnetic quantum number*,  $m$ .

**B-coefficient** (B3: 216) Another term for the *Einstein B-coefficient*.

**band gap** (B3: 174, 189) In general, a band gap is any gap in *energy* between two *energy bands*. However, the band gap of a *semiconductor* or *insulator* invariably refers to the energy gap between the *valence band* and the *conduction band*.

**band structure** (B3: 184) This term means either (i) the pattern of curves  $E(\mathbf{k})$  of the *energies* of *electrons* in *Bloch wave states* against *wave vector* in a *crystalline solid*, or (ii) the arrangement of *energy bands* in a solid.

**barn** (B1: 196) A unit of area widely used to measure *total cross-sections* in *elementary particle* and nuclear physics.  $1 \text{ barn} = 10^{-28} \text{ m}^2$ .

**barrier penetration** (B1: 88, 133) The quantum phenomenon whereby *particles* may be detected in a *classically-forbidden region*. Compare with *tunnelling*.

**basis** (B2: 12, 17, 206) A set of *vectors* is said to form a basis for a *vector space* if any vector in the space can be expressed as a *linear combination* of vectors from the set. We may also say that the *basis vectors* *span* the vector space or that they are a *complete set*.

The three *Cartesian unit vectors* form a basis for ordinary three-dimensional space. The *ket vectors* corresponding to the *energy eigenfunctions* of a *harmonic oscillator* form a basis for *function space*.

**basis vectors** (B2: 12, 17, 206) The *vectors* in a *basis*. Basis vectors are usually taken to be *normalized* and mutually *orthogonal* (i.e. *orthonormal*).

**BB84 protocol** (B2: 181) A method of *quantum key distribution* that does not rely on *entanglement*. Alice and Bob, who wish to share a *cryptographic key*, each have the same pair of alternative *complementary bases* (e.g the  $H/V$  basis and the *diagonal basis*). Alice chooses one of the bases at random. She measures the *state* of *linear polarization* of a *photon* in this basis, and sends the photon on to Bob. He also randomly chooses one of the bases, and measures the state of linear polarization of Alice's photon in that basis. This is repeated for many photons.

Alice and Bob reject all *measurements* in which

they used different bases. They use a *classical communication channel* to compare their measurements for a subset of the cases where they used the same basis; significant differences indicate the presence of an eavesdropper. If no eavesdropping is detected, the remaining measurements are converted to a binary code to provide a secure shared cryptographic key. Compare with the *Eckert protocol*.

**beam intensity** (B1: 183) For one-dimensional *scattering* and *tunnelling* of a beam of *particles*, the beam intensity is the number of beam particles that pass a given point per unit time. The beam intensity can be identified with the *magnitude* of the corresponding *probability current*. Also called *intensity of a beam*. Compare with *flux* for three-dimensional scattering.

**beam splitter** (B1: 15) A device that splits a beam of *photons* (or other *particles*) into two or more distinct sub-beams. When a single photon passes through a beam splitter, it emerges in a *linear superposition* of the *states* associated with the two output sub-beams, although we cannot say which way the photon went until it is actually detected. A *half-silvered mirror* can be used as a beam splitter.

BOOK 2: *Wollaston prisms* and other devices constructed from *birefringent materials* are used as *polarizing beam splitters*.

**Bell state measurement** (B2: 195) A *measurement* that projects a general *entangled state* of a *system* of two *photons* (or  $\text{spin-}\frac{1}{2}$  *particles*) onto one of the four *Bell states*. After a complete Bell state measurement the system is in the Bell state corresponding to the measurement result, and there is no possibility of finding it in the other three Bell states. Bell state measurements are used in *quantum teleportation*.

**Bell states** (B2: 185) Specific *entangled states* of two *particles*. The four Bell states for the *polarization states* of two *photons* are

$$|\Psi^\pm\rangle = \frac{1}{\sqrt{2}} (|VH\rangle \pm |HV\rangle)$$

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}} (|VV\rangle \pm |HH\rangle),$$

where, for example,  $|VH\rangle$  refers to a *state* in which photon 1 is vertically polarized and photon 2 is horizontally polarized. The Bell states for the *spin states* of two  $\text{spin-}\frac{1}{2}$  *particles* are similar, but with spins replacing polarizations. Bell states are also called *maximally-entangled states*.

**Bell's inequalities** (B2: 162) Inequalities that constrain the possible values of some expressions involving *correlation functions* according to any theory satisfying conditions of *locality* and *realism*; in effect, any theory governed by *local hidden variables*. Bell's inequalities are violated by

some quantum-mechanical predictions, so *local hidden-variable theories* are inconsistent with *quantum mechanics* (*Bell's theorem*). Experiments confirm that Bell's inequalities are violated, and this provides strong evidence against local hidden variables and the notion that *observables* must have definite locally-determined values prior to *measurement*. The *CHSH inequality* is an example of a Bell inequality.

**Bell's theorem** (B2: 162) The theorem stating that no *local hidden-variable theory* can reproduce all the predictions of *quantum mechanics*.

**binding energy** The minimum *energy* needed to separate a *system* into separate *particles*.

**birefringent material** A material such as calcite with an anisotropy axis. *Light* travelling through the material with its *electric field vector* parallel to the anisotropy axis has a different speed to light with its electric field vector perpendicular to the anisotropy axis. Birefringent materials can be used to convert *linearly-polarized light* into *circularly-polarized light* and vice-versa. They can also be used to construct *polarizing beam splitters* such as *Wollaston prisms*.

**bit** (B2: 180) A binary digit that can have only one of two values (0 or 1) corresponding to the two settings of an electrical switch (off or on). A bit is the smallest classical unit of information. Contrast with *qubit*.

**Bloch sphere** An alternative term for the *Poincaré sphere*, but one that is often reserved for the *spin states* of a *spin- $\frac{1}{2}$  particle* rather than the *polarization states* of a *photon*.

**Bloch wave** (B3: 176) An *energy eigenfunction* for an *electron* in an infinite *crystalline solid*. Bloch waves have the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}),$$

where  $\mathbf{k}$  is a *real* quantity called the *wave vector* and  $u_{\mathbf{k}}(\mathbf{r})$  is a function with the *periodicity of the lattice*. A Bloch wave is therefore a modulated *plane wave*.

**Bloch's theorem** (B3: 175) The theorem stating that the *energy eigenfunctions* of the *electrons* in an infinite *crystalline solid* have the *Bloch wave* form

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}),$$

where  $\mathbf{k}$  is a *real* quantity called the *wave vector* and  $u_{\mathbf{k}}(\mathbf{r})$  is a function with the *periodicity of the lattice*.

**Bohm-type experiment** An experiment in which a source prepares a pair of *particles* (e.g. *electrons* or *photons*) in an *entangled state*. The two particles move apart and *measurements* are taken of their entangled attribute (e.g. *spin component* or *linear polarization*). The two measurements are taken at times that are sufficiently close that no signal, travelling at or below the *speed of light* in a vacuum,

can link one measurement event to the other.

Bohm-type experiments are used to test for the violations of *Bell's inequalities* that are predicted by *quantum mechanics*.

**Bohr model** (B3: 37) A semi-quantum model of *atoms* introduced by Niels Bohr in 1913. The model assumes that a central, positively-charged, *nucleus* is orbited by one or more *electrons* that are held in place by *electrostatic forces* given by *Coulomb's law*. It takes the radical step of assuming that only certain stable orbits are possible. Each *Bohr orbit* is characterized by a *quantum number*  $n$  and an *orbital angular momentum* of magnitude  $n\hbar$ , where  $n = 1, 2, 3, \dots$  is a positive integer and  $\hbar$  is *Planck's constant* divided by  $2\pi$ . The model further assumes that electrons do not emit *electromagnetic radiation* as long as they remain in one of the allowed orbits, but that emission (or absorption) of electromagnetic radiation occurs when an electron makes a transition from one orbit to another.

The Bohr model gives reasonable *energy levels* for a *hydrogen atom*:

$$E_n = -\frac{E_R}{n^2},$$

where  $E_R$  is the *Rydberg energy*. Nevertheless, the Bohr model is deeply flawed: it is not consistent with the *Heisenberg uncertainty principle*, it gives the magnitude of the orbital angular momentum in the *ground state* of hydrogen as  $\hbar$  rather than 0, and it cannot be extended successfully to other atoms.

**Bohr orbit** (B3: 37) A stable orbit for an *electron* in the *Bohr model* of an *atom*. For a *hydrogen atom*, a Bohr orbit with *quantum number*  $n$  is a circle of radius  $r_n = n^2 a_0$ , where  $a_0$  is the *Bohr radius*. An electron in this orbit has an *orbital angular momentum* of magnitude  $L = n\hbar$  and a speed  $v_n = e^2 / 4\pi\epsilon_0 \hbar n$  where  $e$  is the magnitude of the electron's *charge*,  $\epsilon_0$  is the *permittivity of free space* and  $\hbar$  is *Planck's constant* divided by  $2\pi$ .

**Bohr radius** (B3: 37) The radius of the lowest *Bohr orbit* in the *Bohr model* of the *hydrogen atom*. Its value is

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{e^2 \mu} = 5.29 \times 10^{-11} \text{ m},$$

where  $e$  is the *magnitude of the charge* of an *electron*,  $\epsilon_0$  is the *permittivity of free space*,  $\hbar$  is *Planck's constant* divided by  $2\pi$  and  $\mu$  is the *reduced mass* of the electron and *proton*.

**Boltzmann distribution law** (B3: 217) The law stating that, in thermal equilibrium at *absolute temperature*  $T$ , the average numbers of *atoms* in *quantum states* 1 and 2, of *energies*  $E_1$  and  $E_2$ , are related by

$$\frac{N_2}{N_1} = \frac{e^{-E_2/kT}}{e^{-E_1/kT}},$$

where  $k$  is Boltzmann's constant.

**Boltzmann's constant** A physical constant  $k$  that relates *absolute temperature to energy*. In SI units,  $k = 1.38 \times 10^{-23} \text{ J K}^{-1}$ .

**bond order** (B3: 163) An abbreviation for *formal bond order*.

**bonding orbital** (B3: 157) A *molecular orbital* with a minimum in its *energy curve* at a value that is lower than either of the *energies* of the *atomic orbitals* from which it is formed. Bonding orbitals have a high *probability density* for *electrons* in the region between *atoms*. Contrast with *antibonding orbital*.

**Born–Oppenheimer approximation** (B3: 144) An approximation that allows us to study the behaviour of the *electrons* in *molecules* and *solids* by treating the *nuclei* as being in fixed positions. The *electronic energy eigenfunctions* and *eigenvalues* are obtained for fixed nuclear positions. The nuclear motions are then obtained by assuming that the electrons adapt instantaneously to each new position of the nuclei, with the *electronic configuration* for each set of fixed nuclear positions contributing to the effective *potential energy function* in which the nuclei move.

In the Born–Oppenheimer approximation, the *time-independent Schrödinger equation* splits into two parts, one for the electrons and the other for the nuclei. These equations are coupled by the fact that the *energy eigenvalues* of the *electronic time-independent Schrödinger equation* depend on the nuclear positions, and these eigenvalues contribute to the *total static energy*, which provides the effective potential energy function in the *nuclear time-independent Schrödinger equation*.

**Born's rule** (B1: 24; B2: 99, 118; B3: 14) For a single *particle* in one dimension, in a *state* described by the *wave function*  $\Psi(x, t)$ , Born's rule tells us that, at time  $t$ , the *probability* of finding the particle in a small interval  $\delta x$ , centred on position  $x$ , is

$$\text{probability} = |\Psi(x, t)|^2 \delta x.$$

For a single particle in three dimensions, in a state described by the wave function  $\Psi(\mathbf{r}, t)$ , the probability, at time  $t$ , of finding the particle in a small volume element  $\delta V$ , centred on position  $\mathbf{r}$ , is

$$\text{probability} = |\Psi(\mathbf{r}, t)|^2 \delta V.$$

BOOK 2: Born's rule can be extended to *systems* of two or more particles. For a one-dimensional system of two *distinguishable particles* in a state described by the wave function  $\Psi(x_1, x_2, t)$ , Born's rule tells us that, at time  $t$ , the probability of finding particle 1 in a small interval  $\delta x_1$ , centred on  $x_1$ , and particle 2 in a small interval  $\delta x_2$ , centred on  $x_2$ , is

$$|\Psi(x_1, x_2, t)|^2 \delta x_1 \delta x_2.$$

Born's rule also applies to systems of *identical particles*. The wave function is then a *symmetric* or *antisymmetric function*, and we interpret  $|\Psi(x_1, x_2, t)|^2 \delta x_1 \delta x_2$  as the probability, at time  $t$ , of finding one particle in a small interval  $\delta x_1$ , centred on  $x_1$ , and another particle in a small interval  $\delta x_2$ , centred on  $x_2$ , irrespective of any labelling convention for the particles.

**Born's rule for momentum** (B1: 170) For a one-dimensional *free-particle wave packet*,

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} A(k) e^{i(kx - E_k t/\hbar)} dk,$$

Born's rule for momentum states that the *probability* of finding the *momentum* to lie in a small interval  $\hbar \delta k$ , centred on  $\hbar k$ , is  $|A(k)|^2 \delta k$ , where  $A(k)$  is called the *momentum amplitude function*.

The *magnitude* of the momentum amplitude function is independent of time for a free particle, but this is not true for a *particle* subject to forces. More generally, Born's rule for momentum states that, at time  $t$ , the probability of finding the momentum to lie in a small interval  $\hbar \delta k$ , centred on  $\hbar k$ , is  $|A(k, t)|^2 \delta k$ , where  $A(k, t)$  is the momentum amplitude function at time  $t$ , given by the *Fourier transform* of the *wave function*:

$$A(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, t) e^{-ikx} dx.$$

Compare with *Born's rule*.

**Bose–Einstein condensate** (B2: 121) A *phase* of matter that occurs at very low temperatures in dilute gases of *boson atoms*. At a critical temperature, a phase transition takes place in which many of the atoms 'condense' into the lowest *energy* single-particle *quantum state*. These atoms form the Bose–Einstein condensate, which behaves in many respects like a single entity, described by a *macroscopic wave function*  $\Psi(\mathbf{r}, t)$ .

**Bose–Einstein condensation** (B2: 121) The process in which a *Bose–Einstein condensate* is formed.

**boson** (B2: 116) A *particle* whose *spin quantum number* is an integer:  $s = 0, 1, 2, \dots$ . Examples include *photons*, *alpha particles* and *deuterons*. A composite particle containing an even number of *fermions* is a boson. A composite particle composed exclusively of bosons is also a boson. A *system* of *identical* bosons is described by a *symmetric total wave function* and is not subject to the *Pauli exclusion principle*. Under suitable conditions, bosons undergo *Bose–Einstein condensation*.

**bound state** (B1: 91) A *state* in which one part of a *system* is always found in close proximity to another part of the same system. The *wave functions* describing bound states are always *normalizable*, and so tend to zero as we move away from the system. The *energy eigenvalues* of bound states are discrete. Contrast with a state in the *continuum*.



**bound system** (B2: 40) A system that is in a *bound state*.

**boundary conditions** (B1: 221) Conditions that give extra information about the solutions of a *differential equation*. Such information may be sufficient to determine all the *arbitrary constants* in the *general solution* of a differential equation, and so select a *particular solution*, or it may determine acceptable *eigenvalues* and *eigenfunctions* that satisfy an *eigenvalue equation*.

**bra vector** (B2: 20) A vector  $\langle g|$  which forms the left-hand part of a *Dirac bracket*  $\langle g|f\rangle$ . Given a *ket vector*  $|g\rangle = \sum_i c_i |g_i\rangle$ , where  $c_i$  are complex constants, the corresponding bra vector is  $\langle g| = \sum_i c_i^* \langle g_i|$ , and this can be joined to any ket vector  $|f\rangle$  to give

$$\langle g|f\rangle = \sum_i c_i^* \langle g_i|f\rangle.$$

The bra vector describing the *spin state* of a *particle* can be represented by a *row spinor*. For example, the row spinor corresponding to  $\langle \uparrow_z |$  is  $[1 \ 0]$ .

**bremsstrahlung** (B3: 99) The continuous *spectrum* of *electromagnetic radiation* from accelerated (taken to include decelerated) charged *particles*. Such radiation is emitted by high-energy *electrons* as they are rapidly brought to rest in the metal target of an *X-ray tube*. Bremsstrahlung means ‘braking radiation’ in German.

**Cartesian coordinate system** (B2: 206) A set of three mutually perpendicular axes pointing outwards from a single origin. The axes are called the *x*-axis, the *y*-axis and the *z*-axis. Such a coordinate system is usually chosen to be right-handed so that, if the fingers of the right hand initially point in the *x*-direction, and are then bent to point in the *y*-direction, the outstretched right thumb points in the *z*-direction.

**Cartesian coordinates** Coordinates *x*, *y* and *z* that represent the position of a point relative to a given *Cartesian coordinate system*.

**Cartesian form** (B1: 213) A *complex number* *z* is said to be expressed in Cartesian form if it is written as  $z = x + iy$ , where *x* and *y* are *real numbers*.

**Cartesian unit vectors** (B2: 42) The three *unit vectors*  $\mathbf{e}_x$ ,  $\mathbf{e}_y$  and  $\mathbf{e}_z$  that point in the directions of the axes of a *Cartesian coordinate system*. This set of *vectors* forms an *orthonormal basis* in ordinary three-dimensional space.

**Cauchy–Schwarz inequality** (B2: 17, 208) An inequality for the *inner product* of two *abstract vectors*  $|f\rangle$  and  $|g\rangle$  in a *vector space*:

$$\langle f|f\rangle \langle g|g\rangle \geq |\langle f|g\rangle|^2.$$

The Cauchy–Schwarz inequality is the starting point for the proof of the *generalized uncertainty principle*.

**central force** (B2: 40) A force between two *particles* that is directed along the line between the two particles and has a *magnitude* that depends only on the distance between the particles. Such a force can be derived from a *spherically-symmetric potential energy function*  $V(r)$ . The *Coulomb force* between two *charges* is central, and so is the gravitational force between a planet and a star.

**central-field approximation** (B3: 124) An approximation for many-electron *atoms* in which the repulsive electron–electron *potential energy functions* in the many-electron *Hamiltonian operator* are replaced by a sum  $\sum_i U_i(r_i)$  of *spherically-symmetric effective potential energy functions* for the individual *electrons*. The Hamiltonian operator for the whole atom is then the sum of spherically-symmetric Hamiltonian operators for the individual electrons. The *time-independent Schrödinger equation* for the whole atom is *separable*, and its solutions can be expressed as products of single-particle *atomic orbitals*, obtained by solving single-particle time-independent Schrödinger equations for the individual electrons. Each atomic orbital is a product of a *radial function* and a *spherical harmonic*.

**centre of symmetry** (B3: 158) A point which, when chosen as origin, allows the *inversion operation*  $\mathbf{r} \rightarrow -\mathbf{r}$  to produce no change in the *Hamiltonian operator* of a given system. All *homonuclear diatomic molecules* have a centre of symmetry midway between the *nuclei*.

**centre-of-mass frame** (B1: 127) A *frame of reference* whose origin permanently coincides with the centre of mass of a given system of *particles*.

**centrifugal barrier** (B3: 18) An effective *potential energy barrier* for a *particle* in a *spherically-symmetric potential energy well*. The centrifugal barrier appears in the *radial equation*, and takes the form  $l(l+1)/2\mu r^2$  for a particle of *reduced mass*  $\mu$  in a state with *orbital angular momentum quantum number* *l*.

**chain rule of partial differentiation** (B2: 50) A mathematical rule for *partial derivatives*. If *f* is a function of *x*, *y* and *z*, each of which is a function of *r*,  $\theta$  and  $\phi$ , the chain rule states that

$$\frac{\partial f}{\partial \phi} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial \phi} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \phi} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \phi},$$

with similar results for  $\partial f/\partial \theta$  and  $\partial f/\partial r$ .

**characteristic equation** (B2: 224) The equation

$$\det(\mathbf{A} - \lambda \mathbf{I}) = 0,$$

where *A* is an  $n \times n$  *square matrix*, *I* is an  $n \times n$  *unit matrix* and  $\lambda$  is a *scalar*. When the *determinant* on the left-hand side is expanded, the solutions of the resulting polynomial equation are the *eigenvalues* of the matrix *A*.

**charge** Often used as an abbreviation for *electric charge*.

**charmonium** (B3: 112) A *bound state* of a heavy *quark* and an antiquark, which has some of the properties of a *hydrogen-like system*.

**chemical element** A specific type of *atom*, characterized by a particular *atomic number*  $Z$ . The *nucleus* of the atom contains  $Z$  *protons*, and a neutral atom contains  $Z$  *electrons*. Different *isotopes* of an element have different atomic masses because of different numbers of *neutrons* in their nuclei, but all isotopes of the same element have the same chemical properties.

**CHSH inequality** (B2: 162) One of *Bell's inequalities* that is well-adapted to the comparison of theory with experiment. In a *Bohm-type experiment*, the CHSH inequality takes the form

$$|\Sigma| \leq 2,$$

where

$\Sigma = C(\theta_1 - \theta_2) + C(\theta_1 - \theta'_2) + C(\theta'_1 - \theta_2) - C(\theta'_1 - \theta'_2)$ , and  $C(\theta_1 - \theta_2)$  is a *correlation function* for *measurements* taken with the detector 1 oriented at  $\theta_1$  and detector 2 oriented at  $\theta_2$ .

The fact that *quantum mechanics* predicts violations of the CHSH inequality leads directly to *Bell's theorem*. The fact that experiments confirm violations of the CHSH inequality is strong evidence against *local hidden-variable theories*.

**ciphertext** (B2: 180) An encrypted message. Also called a *cryptogram*.

**circular polarization** (B2: 166) In *classical physics*, *light* has circular polarization if its *electric field vector* maintains a fixed *magnitude* and rotates at a constant rate about the direction of propagation. In the convention adopted in optics, and in this course, light has *right-handed circular polarization* if the rotation is clockwise as seen by an observer looking towards to source; it has *left-handed circular polarization* if the rotation is anticlockwise as seen by an observer looking towards to source.

In *quantum mechanics*, a *photon* with right-handed circular polarization has an *angular momentum component*  $-\hbar$  along its direction of propagation and its *polarization state* is

$$|R\rangle = -\frac{1}{\sqrt{2}}(|H\rangle + i|V\rangle),$$

where  $|H\rangle$  is a *state* of *horizontal polarization* and  $|V\rangle$  is a *state* of *vertical polarization*.

A photon with left-handed circular polarization has an angular momentum component  $+\hbar$  along its direction of propagation and its polarization state is

$$|L\rangle = \frac{1}{\sqrt{2}}(|H\rangle - i|V\rangle).$$

**circularly polarized** The condition of having *circular polarization*.

**classical communication channel** (B2: 181) A communication channel using macroscopic phenomena, such as the flow of an *electric current* in an ordinary wire or the transmission of *light*, in which vast numbers of incoherent *electrons* or *photons* are involved rather than single *particles*. Classical communication channels can be used in conjunction with *quantum communication channels* in *protocols* for *quantum key distribution* and *quantum teleportation*.

**classical limit** (B1: 160) Limiting conditions under which the predictions of *quantum mechanics* approach those of *classical mechanics*. The classical limit generally involves objects that are much larger than *atoms*, and forces that vary slowly over the width of the *wave packet* describing the object. See also the *correspondence principle* and *Ehrenfest's theorem*.

**classical mechanics** A theory of the behaviour of *systems* of *particles* based on Newton's laws. Fundamental equations in classical mechanics can be expressed in terms of the *Hamiltonian function*. Also called Newtonian mechanics.

**classical physics** (B1: 7) A term given to branches of physics that do not rely on quantum ideas. Classical physics embraces *classical mechanics* and subjects such as classical electromagnetism, fluid mechanics and thermodynamics. Most physicists regard special and general relativity as belonging to classical physics, which implies that the major revolution of twentieth-century physics was *quantum physics*, not relativity.

**classically-forbidden region** (B1: 66) A region of space from which a *particle* is excluded in *classical mechanics*. The exclusion arises because the fixed total *energy* of the particle is less than the value of the *potential energy function* throughout the classically-forbidden region. A classically-forbidden region may be accessible in *quantum mechanics* through the phenomenon of *barrier penetration*.

**closed shell** (B3: 127) A *shell* that cannot contain any more *electrons*. For example s-, p-, d- and f-shells are closed if they contain 2, 6, 10 and 14 electrons respectively. Contrast with *open shell*.

**coefficient rule** (B1: 105) This rule states that, if the *wave function*  $\Psi(x, t)$  of a *system* is expressed as a discrete *linear combination* of *normalized energy eigenfunctions*:

$$\Psi(x, t) = c_1(t) \psi_1(x) + c_2(t) \psi_2(x) + \dots,$$

then the *probability* of obtaining the  $i$ th *energy eigenvalue*  $E_i$  is

$$p_i = |c_i(t)|^2,$$



where  $c_i(t)$  is the coefficient of the  $i$ th energy eigenfunction in the wave function at the instant of *measurement*.

This rule can be extended to any *observable*,  $A$ , with a discrete set of values provided that the wave function is expanded as a linear combination of *eigenfunctions* of the corresponding quantum-mechanical operator  $\hat{A}$ .

BOOK 2: The coefficient rule can also be expressed in *Dirac notation*. If the *state vector* of a system is expressed as

$$|\Psi\rangle = \sum_i c_i |\phi_i\rangle,$$

where  $|\phi_i\rangle$  is an *eigenvector* of the operator  $\hat{A}$  with discrete eigenvalue  $a_i$ , the probability that a measurement of  $A$  in the *state*  $|\Psi\rangle$  will give the value  $a_i$  is  $|c_i|^2$ .

**cofactor** (B2: 222) The cofactor of a given element  $A_{ij}$  in a *determinant* or a *matrix*  $A$  is found by striking out the row and column that contain the given element, forming the determinant of the remaining elements in the order that they appear in the original determinant or matrix, and then multiplying the result by  $(-1)^{i+j}$ , where  $i$  and  $j$  are the row and column numbers of the given element.

Cofactors are used to evaluate *determinants* and to find the inverse of a *square matrix*.

**coherent waves** Two *waves* are said to be coherent with one another if knowledge of the *phase* of one wave at a particular position and time enables the phase of the other wave to be predicted at some other position and time.

**cohesive energy** The minimum amount of *energy* needed to separate a solid into separate *atoms*.

**collapse of the state vector** (B2: 86, 136) A sudden and abrupt change in the *state* of a *quantum system* that occurs when a *measurement* is made. This collapse cannot be described by *Schrödinger's equation*. If a measurement of the *observable*  $A$  yields the discrete value  $a_i$ , the state of the system immediately after the measurement is described by the *eigenfunction* or *eigenvector* of  $\hat{A}$  with *eigenvalue*  $a_i$ .

For example, in the case of a measurement of the *spin component*  $S_n$  of a *spin- $\frac{1}{2}$  particle*, the *spin state* prior to the measurement may be a *linear combination* of  $|\uparrow_n\rangle$  and  $|\downarrow_n\rangle$ , the eigenvectors of the *general spin matrix*  $\hat{S}_n$ . Immediately after the measurement, the spin state of the *particle* is represented by  $|\uparrow_n\rangle$  if the measured value was  $+\hbar/2$ , and  $|\downarrow_n\rangle$  if the measured value was  $-\hbar/2$ .

**collapse of the wave function** (B1: 27, 97) The abrupt and unpredictable change in a *wave function* that arises during an act of *measurement*. This

collapse cannot be described by *Schrödinger's equation*. An example is the collapse that occurs when the position of a *particle* is measured by a *Geiger counter*; immediately after the Geiger counter has clicked, the wave function describing the particle is localized in the vicinity of the Geiger counter.

**column matrix** (B2: 215) A *matrix* with a single column.

**column spinor** (B2: 78) A *column matrix* used to represent a *spin ket vector*.

**commutation relation** (B1: 138; B2: 28) An equation for the *commutator* of two given *operators*. For example, the *lowering* and *raising operators* of a *harmonic oscillator* obey the commutation relation

$$[\hat{A}, \hat{A}^\dagger] = 1.$$

BOOK 2: Other important commutation relations include

$$[\hat{x}, \hat{p}_x] = i\hbar \quad \text{and} \quad [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z.$$

for the *position operator*  $\hat{x}$ , the *momentum operator*  $\hat{p}_x$  and the *angular momentum operators*  $\hat{L}_x$ ,  $\hat{L}_y$  and  $\hat{L}_z$ .

**commutator** (B1: 138; B2: 27) The commutator of two *operators*  $\hat{A}$  and  $\hat{B}$  is itself an operator, denoted by the symbol  $[\hat{A}, \hat{B}]$ , and defined by

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}.$$

See also *commuting operators*.

**commute** (B2: 27, 217) See *commuting operators*.

**commuting operators** Two *operators*  $\hat{A}$  and  $\hat{B}$  *commute* with each other if they have the same effect no matter which order they are applied. The result of operating on a function  $f(x)$  with  $\hat{A}$  followed by  $\hat{B}$  is  $\hat{B}\hat{A}f(x)$ , while the result of operating on  $f(x)$  with  $\hat{B}$  followed by  $\hat{A}$  is  $\hat{A}\hat{B}f(x)$ . For commuting operators, these two results are always the same, for all functions  $f(x)$ . We then write

$$\hat{A}\hat{B} = \hat{B}\hat{A}.$$

Equivalently,

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0,$$

so the *commutator* of two commuting operators is equal to zero.

**compatible observables** (B2: 59) Two *observables*  $A$  and  $B$  are said to be compatible with one another if they can simultaneously have definite values in the same *quantum state* (for a range of different values). For this to happen, the quantum-mechanical *operators*  $\hat{A}$  and  $\hat{B}$  must *commute* with one another so that a set of simultaneous *eigenfunctions* (or *eigenvectors*) exists.

Conversely, if  $A$  and  $B$  have discrete values, and  $\hat{A}$  and  $\hat{B}$  commute with one another, then

these observables are compatible. Contrast with *incompatible observables*.

**complementary bases** (B2: 179) A

two-dimensional *basis* ( $|a_1\rangle, |a_2\rangle$ ) is said to be complementary to another two-dimensional basis ( $|b_1\rangle, |b_2\rangle$ ) if each *basis vector* in the first basis has projections of equal *magnitude* onto the two basis vectors of the second basis:

$$|\langle a_1|b_1\rangle| = |\langle a_1|b_2\rangle| = \frac{1}{\sqrt{2}}$$

$$|\langle a_2|b_1\rangle| = |\langle a_2|b_2\rangle| = \frac{1}{\sqrt{2}}.$$

Suppose that *observable A* has two possible values,  $a_1$  and  $a_2$ , corresponding to the *eigenvectors*  $|a_1\rangle$  and  $|a_2\rangle$ , and *observable B* has two possible values,  $b_1$  and  $b_2$ , corresponding to the eigenvectors  $|b_1\rangle$  and  $|b_2\rangle$ . Then the complementary relationship between the two bases implies that the *states*  $|a_1\rangle$  and  $|a_2\rangle$  each have definite values of *A*, but equal *probabilities* for the two possible values of *B*. Similarly, the states  $|b_1\rangle$  and  $|b_2\rangle$  each have definite values of *B*, but equal probabilities for the two possible values of *A*. This property makes complementary bases suitable for the BB84 protocol of quantum key distribution.

**complete set of functions** (B1: 164; B2: 11) A discrete set of functions,  $\phi_i(x)$  labelled by the index  $i = 0, 1, 2, \dots$ , is said to be complete if it is possible to expand any reasonable function  $f(x)$  in the form

$$f(x) = \sum_{i=0}^{\infty} c_i \phi_i(x),$$

where the coefficients  $c_i$  are constants (possibly *complex*, but independent of  $x$ ). The *harmonic-oscillator energy eigenfunctions* are complete in this sense.

This definition is extended to a continuous set of functions  $\phi_k(x)$ , labelled by a continuous index  $k$ , by replacing the sum by an integral:

$$f(x) = \int_{-\infty}^{\infty} C(k) \phi_k(x) dk,$$

where  $C(k)$  is some complex-valued function. The *momentum eigenfunctions* are complete in this sense.

**complete set of outcomes** (B1: 228) A set of *mutually exclusive outcomes* for an experiment is said to be complete if every possible outcome of the experiment is a member of the set.

**complete set of vectors** (B2: 17) In a given *vector space*, a set of *vectors* is said to be complete if it is possible to express any vector in the space as a *linear combination* of vectors from the set. We may also say that the vectors *span* the space, or that they provide a *basis* for it.

**complex conjugate** (B1: 212) For a given *complex number*  $z$ , the complex conjugate  $z^*$  is the complex

number obtained by reversing the sign of  $i$  wherever it appears in  $z$ . So, given a complex number

$$z = x + iy = r(\cos \theta + i \sin \theta) = re^{i\theta},$$

where  $x, y, r$  and  $\theta$  are *real*, the complex conjugate of  $z$  is

$$z^* = x - iy = r(\cos \theta - i \sin \theta) = re^{-i\theta}.$$

**complex number** (B1: 210) An entity that can be written in the form

$$z = x + iy,$$

where  $x$  and  $y$  are *real numbers* and  $i = \sqrt{-1}$ .

Complex numbers obey the ordinary rules of algebra, with the extra rule that  $i^2 = -1$ . See also *polar form*, *exponential form*, *argument*, *phase* and *complex conjugate*.

**complex plane** (B1: 212) A plane in which *complex numbers* in the *Cartesian form*  $z = x + iy$  are represented by points with *Cartesian coordinates*  $(x, y)$ . *Real numbers* are represented by points along the (horizontal)  $x$ -axis, and *imaginary numbers* are represented by points along the (vertical)  $y$ -axis. Also called the *Argand diagram*.

**component** (B2: 12, 17, 206) The component of a *vector* along a given axis is the *magnitude* of the vector times the cosine of the angle between the direction of the vector and the direction the axis. Components can be positive, negative or zero.

When a vector  $\mathbf{a}$ , is expressed as a *linear combination* of *Cartesian unit vectors*  $\mathbf{e}_x, \mathbf{e}_y$  and  $\mathbf{e}_z$ :

$$\mathbf{a} = a_x \mathbf{e}_x + a_y \mathbf{e}_y + a_z \mathbf{e}_z,$$

the *scalar coefficients*  $a_x, a_y$  and  $a_z$  are the components of the vector  $\mathbf{a}$ . In geometric terms, the component  $a_x$  is found by projecting  $\mathbf{a}$  onto the  $x$ -axis.

BOOK 2: This definition can be extended to *vectors* an abstract *vector space*. If  $|a\rangle$  is expressed as a linear combination of basis vectors  $|e_i\rangle$ :

$$|a\rangle = \sum_i a_i |e_i\rangle,$$

the scalar coefficients  $a_i$  are the components of the vector. If the *basis vectors* are *orthonormal*, we have

$$a_i = \langle e_i | a \rangle.$$

**condensate** A shorthand term for *Bose–Einstein condensate*.

**conduction band** (B3: 189) In a *semiconductor* or *insulator*, the conduction band is the lowest *energy band* that is unoccupied at *absolute zero*. At non-zero temperatures, the conduction band of a semiconductor is occupied by a small number of *electrons* as a result of thermal excitation from the *valence band* or from

*donor atom states* just below the conduction band. Contrast with *valence band*.

**conductivity** Often used as an abbreviation for *electrical conductivity*.

**conductor** (B3: 186) In the context of electrical conduction, a conductor is a material that has a high *electrical conductivity*. Conductors have a partly-full *energy band* at the *absolute zero* of temperature. Contrast with *insulator* and *semiconductor*.

**configuration** (B3: 126, 162) Often used as an abbreviation for *electronic configuration*.

**conservation of energy** (B1: 105) The principle that the total *energy* of any *isolated system* remains constant in time. In applying this principle, it is essential to include the energies of any *photons* that are absorbed or emitted.

In *quantum physics*, where a system may have an indefinite energy, conservation of energy is the principle that the *probability distribution* of energy, in any isolated system, remains constant in time. It then follows that the *expectation value* and the *uncertainty* of the energy remain constant in time.

**conserved quantities** In a given *system*, a quantity *A* is conserved if the corresponding quantum-mechanical *operator*  $\hat{A}$  commutes with the *Hamiltonian operator* for the system. The *generalized Ehrenfest theorem* then shows that the *expectation value* of *A*, and the *uncertainty* of *A* remain constant in time.

**constructive interference** (B1: 28) The phenomenon in which two or more *waves* reinforce one another when they are superimposed at a given point. Contrast with *destructive interference*.

**continuity boundary conditions** (B1: 68) *Boundary conditions* that refer to the continuity of *energy eigenfunctions* and their derivatives. The energy eigenfunction  $\psi(x)$  is always continuous. The first derivative  $d\psi/dx$  is continuous in regions where the *potential energy function* is finite; it need not be continuous at points where the potential energy function becomes infinite. Note that *wave packets* composed of an infinite number of energy eigenfunctions are not subject to continuity boundary conditions.

**continuous probability distribution** (B1: 231) A *probability distribution* for a continuous *random variable*, specified by an appropriate *probability density function*.

**continuum** (B1: 12) (i) The name given to an infinite set of *energy levels* over which the *energy* varies continuously. The *state* of a *particle* in the continuum cannot be described by a *stationary-state wave function* of definite energy because such a function cannot be *normalized*; instead, it is described

by a *wave packet* of indefinite energy.

(ii) In mathematics, any continuous set of values (as opposed to a discrete set of values) is said to form a continuum.

**correlation function** (B2: 160) In the context of *Bohm-type experiments*, a correlation function is a function  $C(\theta_1, \theta_2)$  of the angles  $\theta_1$  and  $\theta_2$  that specify the orientations of the two detectors relative to fixed coordinate system. It is the *probability* that the two detectors will give similar results, minus the probability that they will give dissimilar results.

For experiments carried out with *photons*, ‘similar results’ means that, relative to their own orientations, both detectors register *vertical polarization*, or both register *horizontal polarization*. For experiments carried out with *spin- $\frac{1}{2}$  particles*, ‘similar results’ means that, relative to their own orientations, both detectors register *spin-up*, or both register *spin-down*. For some *entangled states* (e.g. the *singlet state* of two spin- $\frac{1}{2}$  particles) the correlation function depends only on the difference of the two angles, and is written as  $C(\theta_1 - \theta_2)$ .

Correlation functions appear in *Bell’s inequalities*, including the *CHSH inequality*.

**correspondence principle** (B1: 135) The general principle that the predictions of *quantum mechanics* should approach those of *classical mechanics* in the limit of high *quantum numbers*. See also *classical limit*.

**$\cos^2(\theta/2)$  rule** (B2: 69) The rule stating that a *spin- $\frac{1}{2}$  particle* that is transmitted through one *Stern–Gerlach apparatus*, has a *probability*  $\cos^2(\theta/2)$  of passing through a second Stern–Gerlach apparatus oriented at an angle  $\theta$  relative to the first. Compare with *Malus’s law*.

**Coulomb barrier** (B1: 204) The repulsive barrier, described by the *Coulomb potential energy function*

$$V(r) = \frac{Qq}{4\pi\epsilon_0 r},$$

that is encountered by a *particle* of charge *q* when it is a distance *r* from a fixed point-like charge *Q*, where *q* and *Q* have the same sign. (If *q* and *Q* have opposite signs, the repulsive barrier becomes an attractive well.)

**Coulomb force** The *electrostatic force* between two charged *particles*, given by *Coulomb’s law*.

**Coulomb integral** (B3: 122) An integral of the form

$$C_{rs} = \frac{e^2}{4\pi\epsilon_0} \iint \frac{|\phi_r(\mathbf{r}_1)|^2 |\phi_s(\mathbf{r}_2)|^2}{r_{12}} dV_1 dV_2$$

that partly describes the average *Coulomb potential energy* of two *electrons* occupying orbitals  $\phi_r$  and  $\phi_s$  in an *atom* or *molecule*. Because the electrons are *indistinguishable particles*, the contribution of the *exchange integral* must also be considered.



**Coulomb model** (B3: 35) A model of the *hydrogen atom* that treats the *electron* and *proton* as point-like *particles* interacting only via the *Coulomb force*.

The Coulomb model ignores the *spin-orbit interaction*, relativistic modifications to the *kinetic energy*, the *Darwin term*, coupling between the *spins* of the proton and the electron, the finite size of the proton, and *quantum field theory* effects such as the *Lamb shift*. The Coulomb model accounts for the gross structure of the hydrogen atom *spectrum*, but not for its *fine structure* or *hyperfine structure*.

**Coulomb potential energy function** A function specifying the mutual *potential energy* of two charged *particles* in a vacuum. This is given by

$$E_{\text{pot}} = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r},$$

where  $q_1$  and  $q_2$  are the *charges* of the particles,  $r$  is their separation and  $\epsilon_0$  is the *permittivity of free space*. By convention, the *zero of potential energy* is taken to correspond to infinite separation of the particles, so the Coulomb potential energy of oppositely-charged particles is negative.

**Coulomb's law** The physical law quantifying the *electrostatic force* between two stationary charged *particles*. This force acts along the line joining the particles; it is repulsive if the *charges* have the same sign and attractive if they have opposite signs. The force has *magnitude*

$$F = \frac{1}{4\pi\epsilon_0} \frac{|q_1 q_2|}{r^2},$$

where  $q_1$  and  $q_2$  are the charges of the particles,  $r$  is the distance between them and  $\epsilon_0$  is the *permittivity of free space*.

**covalent bonding** (B3: 171) Bonding in which *electrons* occupy mainly *bonding orbitals* between neighbouring *atoms*, and in which significant electron *probability density* is found in regions between atoms. Contrast with *ionic bonding* and *metallic bonding*.

**cryptogram** (B2: 180) An encrypted message. Also called a *ciphertext*.

**cryptographic key** (B2: 180) A sequence of binary digits used to encrypt a message. The cryptographic key is combined with the *plaintext* message to render the message undecipherable to anyone who intercepts the message but doesn't have the cryptographic key.

**crystal** An alternative term for *crystalline solid*.

**crystal lattice** See *lattice*.

**crystalline solid** (B3: 169) A solid in which a particular arrangement of *atoms* is repeated over a regular three-dimensional grid called a *lattice*. In simple cases, the repeat unit is a single atom and all atoms in an infinite crystal have equivalent environments.

**crystalline structure** See *crystalline solid*.

**current** An abbreviation for *electric current*.

**current density** (B3: 189) A *vector* quantity  $\mathbf{J}$  that points in the direction of *electric current* flow, with a *magnitude* equal to the *current* per unit cross-sectional area perpendicular to the flow. The *SI* unit of current density is  $\text{A m}^{-2}$ .

**cycle** The shortest part of an *oscillation* or *wave* over which the motion repeats itself; a cycle endures for exactly one *period*.

**Darwin term** (B3: 106) A small *perturbation* to the *Hamiltonian operator* of a *hydrogen atom* that modifies the *energy* of *quantum states* with  $l = 0$ , where  $l$  is the *orbital angular momentum quantum number*. The Darwin term arises in a fully-relativistic treatment and its effect is calculated using *time-independent perturbation theory*.

**de Broglie relationship** (B1: 21) The relationship between the *de Broglie wavelength*  $\lambda_{\text{dB}}$  and the *magnitude*  $p$  of the *momentum* of a *free particle*:

$$\lambda_{\text{dB}} = \frac{h}{p},$$

where  $h$  is *Planck's constant*.

**de Broglie wave** A *wave* used in *quantum physics* to describe a *free particle*.

**de Broglie wave function** (B1: 27) A *wave function* of the form  $Ae^{i(kx-\omega t)}$  that describes a *stationary state* of a *free particle* in *quantum mechanics*. This is a *wave* of *amplitude*  $|A|$ , propagating in the  $x$ -direction with *wave number*  $k$  and *angular frequency*  $\omega$ , corresponding to a free particle with *momentum*  $p_x = \hbar k$  and *energy*  $E = \hbar\omega$ .

A de Broglie wave function does not describe a fully-realistic *quantum state* because it cannot be *normalized*, but realistic wave functions for free particles can be formed by taking continuous *linear combinations* of de Broglie wave functions (free-particle *wave packets*).

**de Broglie wavelength** (B1: 21) The *wavelength* of a *de Broglie wave*, given by the *de Broglie relationship*,  $\lambda_{\text{dB}} = h/p$ .

**decay constant** (B1: 13) A quantity,  $\lambda$ , with units of inverse time, characterizing the *radioactive decay* of a specific kind of *nucleus* (or the *particle decay* of a specific kind of *particle*). The *probability* of decay in a short time interval  $\delta t$  is  $\lambda \delta t$ , which is independent of time. Given a large sample of nuclei of the same kind, the average number of nuclei that remain undecayed at time  $t$  falls exponentially according to the *exponential law of radioactive decay*,

$$N(t) = N(0) e^{-\lambda t}.$$

where  $N(0)$  is the initial number of nuclei at time  $t = 0$ . See also *half-life*.

**degeneracy** (B1: 81) The occurrence of different *quantum states* with the same *energy*.

**degenerate** (B1: 81) Two *quantum states* are said to be degenerate with one another if they have the same *energy*. An *energy level* that corresponds to more than one quantum state is also said to be degenerate.

**dependent variable** In a function  $f(x, y, \dots, z)$ , the dependent variable is  $f$ . Contrast with the *independent variables*  $x, y, \dots, z$ .

**destructive interference** (B1: 28) The phenomenon in which two or more *waves* cancel one another when they are superimposed at a given point. Contrast with *constructive interference*.

**determinant** (B2: 41, 222) A shorthand notation for a particular *linear combination* of products of terms (*elements* of the determinant). The determinant is presented as a square array of elements and is evaluated by selecting any complete row or column and taking the sum of all the elements in that row or column, multiplied by their corresponding *cofactors*.

For example, the *vector product*  $\mathbf{a} \times \mathbf{b}$  is given by the determinant

$$\begin{vmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} = (a_y b_z - a_z b_y) \mathbf{e}_x - (a_x b_z - a_z b_x) \mathbf{e}_y + (a_x b_y - a_y b_x) \mathbf{e}_z.$$

Determinants also appear in the *characteristic equation* that gives the *eigenvalues* of *square matrices*.

**deterministic** (B1: 13) A term indicating that identical *initial conditions* lead to identical outcomes on all occasions. For example, *classical mechanics* is a deterministic theory. Contrast with *indeterministic*.

**deuterium atom** An *isotope* of *hydrogen* with *mass number*  $A = 2$ . A neutral deuterium atom has a single *electron* outside a deuterium *nucleus*, which consists of a *bound state* of a *proton* and a *neutron* (a *deuteron*).

**deuteron** (B1: 91) A *bound state* of a *proton* and a *neutron*. A deuteron is the *nucleus* of a *deuterium atom*.

**diagonal basis** (B2: 178) A *basis* representing the *polarization states* of *photons* in which the *basis vectors* correspond to photons *linearly polarized* at  $45^\circ$  to the vertical and horizontal. This is a *complementary basis* to the  $H/V$  basis.

**diatomic molecule** A *molecule* consisting of two *atoms* bound together.

**differential cross-section** (B1: 196) A quantity used to measure the rate per unit incident *flux* per unit solid angle, at which a given type of target scatters a given type of incident *particle* into a small cone of angles around a specified direction. The integral of the

differential cross-section over all directions is equal to the *total cross-section*. Compare with *reflection coefficient* in one dimension.

**differential equation** (B1: 217) An equation that involves derivatives of a function. *Ordinary differential equations* involve ordinary derivatives, while *partial differential equations* involve *partial derivatives*. However, the term ‘differential equation’ is often used as a shorthand for ‘ordinary differential equation’. The process of solving the differential equation involves finding functions that satisfy the equation. We may be interested in finding *general solutions*, or finding *particular solutions* that satisfy the equation together with appropriate *boundary conditions* or *initial conditions*.

**diffraction** (B1: 16) The spreading of a *wave* that occurs when it passes through an aperture or around an obstacle. Diffraction is caused by the *interference* of waves taking different routes. Classical examples include the diffraction of water waves, sound waves and *light waves*. In *quantum mechanics*, the wave could be the *wave function* that describes an *electron* propagating according to *Schrödinger’s equation* after passing through a narrow slit.

**diffraction pattern** (B1: 18) The *intensity pattern* of a *wave* that has been diffracted after passing through an aperture or around an obstacle. The *diffraction* arises as a result of *interference*, so the diffraction pattern generally displays *interference maxima* and *interference minima*.

**Dirac bracket** (B2: 14) In *wave mechanics*, the Dirac bracket of two functions  $f(x)$  and  $g(x)$  is a *complex number* defined by the *overlap integral* of  $f(x)$  and  $g(x)$ :

$$\langle f|g \rangle = \int_{-\infty}^{\infty} f^*(x) g(x) dx.$$

For two functions  $f(x, y, z)$  and  $g(x, y, z)$ , the definition is extended to give

$$\langle f|g \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f^*(x, y, z) g(x, y, z) dx dy dz.$$

The Dirac bracket provides an *inner product* for *function space*.

Dirac brackets obey the rules:

$$\langle f|g \rangle = \langle g|f \rangle^*$$

$$\langle f|f \rangle \geq 0$$

$$\langle f|\sum_i c_i g_i \rangle = \sum_i c_i \langle f|g_i \rangle$$

$$\langle \sum_i c_i g_i|f \rangle = \sum_i c_i^* \langle g_i|f \rangle$$

and the *Cauchy–Schwarz inequality*.

**Dirac equation** (B3: 108) A relativistic quantum-mechanical *partial differential equation* that describes the behaviour of *spin- $\frac{1}{2}$  particles*. The equation involves a  $4 \times 4$  *matrix operator* whose *elements* involve *first-order partial derivative operators* with respect to space and time coordinates; this acts on a  $4 \times 1$  *spinor wave function*.

The Dirac equation accounts for the *magnetic dipole moment* of the *electron*, the *fine structure* of the *hydrogen atom spectrum* and the existence of *positrons*. While the Dirac equation is an advance on the non-relativistic *Schrödinger equation*, it is itself superseded by *quantum field theory*.

**Dirac notation** (B2: 14) A notation invented by Dirac which uses the symbol  $\langle f|g \rangle$  for the *inner product* of two *abstract vectors*. The symbols  $\langle f|$  and  $|g \rangle$  can be treated separately and are referred to as *bra* and *ket vectors*, respectively.

**dissociation energy** The minimum *energy* needed to split a *molecule* into separate *atoms*, starting with the molecule in its lowest vibrational *state*. In the electronic *ground state* of the molecule, the dissociation energy is equal to the *spectroscopic dissociation energy* minus the *zero-point energy* of vibrations.

**distinguishable particles** *Particles* that can be meaningfully labelled, allowing us to say that particle 1 is distinct from particle 2. So, if we find a particle at a given place, we can tell whether it is particle 1 or particle 2. Contrast with *indistinguishable particles*.

**donor atom** (B3: 191) A type of impurity *atom* in a *semiconductor* that can donate *electrons* to the *conduction band* of the semiconductor. With a sufficient *number density* of donor atoms an *n-type semiconductor* can be produced. Donor atoms for silicon or germanium include phosphorus, arsenic and antimony in *Group 15* of the *Periodic Table*. Contrast with *acceptor atom*.

**doped semiconductor** See *doping*.

**doping** (B3: 190) The process of deliberately adding impurities to a *semiconductor* to change its electrical properties. *Donor atoms* may be added to increase the number of *electrons* in the *conduction band*, or *acceptor atoms* may be added to increase the number of *holes* in the *valence band*. If doping is at a sufficient concentration, *n-type semiconductors* and *p-type semiconductors* can be produced with donor and acceptor atoms, respectively.

**double bond** (B3: 163) In the *LCAO approximation* for *molecules*, a chemical bond with a *formal bond order* of 2 is referred to as a double bond.

**dummy index** (B2: 217) An index internal to an expression that can be given a different label without affecting the meaning the expression.

**Eckert protocol** (B2: 184) A method of *quantum key distribution* that uses *entanglement* to allow two people, Alice and Bob, to share a *cryptographic key*, checking whether any eavesdropping has taken place. A source creates a pair of *photons* in a particular *entangled polarization state*. One of the photons is sent to Alice and other to Bob, each of whom measures the *linear polarization* of their photon in one of three *bases* chosen randomly and independently. This procedure is repeated for many pairs of photons.

When Alice and Bob choose the same basis, their results are perfectly correlated or anticorrelated (depending on the choice of entangled state); these results are used to provide a shared cryptographic key. The three bases are oriented in such a way that, when Alice and Bob choose particular combinations of different bases, an entangled state will exhibit *non-local effects* that violate the *CHSH inequality*. On average, this should happen in about half the cases where different bases are used. An eavesdropper who takes *measurements* on an entangled photon pair will destroy all non-local correlations. Alice and Bob will therefore be able to detect the presence of the eavesdropper by a reduction in the number of violations of the CHSH inequality. Compare with the *BB84 protocol*.

**effective mass** (B3: 184) In a *crystalline solid*, the *energy* of an *electron* near the bottom of an *energy band* may depend quadratically on the *magnitude*  $k$  of the *wave vector*:

$$E = \frac{\hbar^2 k^2}{2m_e^*}.$$

In this case  $m_e^*$  is called the effective mass of the electron. A similar definition applies to the effective mass of *holes* near the top of the *valence band* of a *semiconductor*.

**Ehrenfest's equations** (B2: 30) Equations describing the rates of change of the *expectation values* of position and *momentum* that appear in *Ehrenfest's theorem*.

**Ehrenfest's theorem** (B1: 158) The theorem stating that the *expectation values* of the position and *momentum* of a single *particle* obey the equations

$$\frac{d\langle x \rangle}{dt} = \frac{\langle p_x \rangle}{m}$$

and

$$\frac{d\langle p_x \rangle}{dt} = - \left\langle \frac{\partial V}{\partial x} \right\rangle,$$

where  $V(x)$  is the *potential energy function* and the expectation values on both sides are evaluated in the same *quantum state*. Ehrenfest's theorem is always true. In the *classical limit*, it helps us to understand how the results of *quantum mechanics* approach those of *classical mechanics*.



BOOK 2: Ehrenfest's theorem is part of a wider result called the *generalized Ehrenfest theorem*, which can be proved using *Schrödinger's equation* and the *Hermitian* nature of the *Hamiltonian operator*.

**eigenfunction** (B1: 43, 221) A function that satisfies an *eigenvalue equation* together with appropriate *boundary conditions*. In *quantum mechanics*, *eigenfunctions* with different *eigenvalues* are mutually *orthogonal*.

**eigenstate** (B2: 60) A *quantum state* that is described by a *eigenfunction* or an *eigenvector* of a given *operator* is said to be an eigenstate of that operator.

**eigenvalue** (B1: 43, 221; B2: 224) In the context of *operators* acting on functions, a particular *scalar*  $\lambda$  is an eigenvalue of the operator  $\hat{A}$  if it permits a solution  $f(x)$  to be found to the *eigenvalue equation*

$$\hat{A}f(x) = \lambda f(x),$$

where  $f(x)$  is not identically equal to zero and is subject to appropriate *boundary conditions*. As a general rule, the eigenvalues of a quantum-mechanical operator  $\hat{A}$  are the only possible outcomes of a *measurement* of the corresponding *observable*,  $A$ .

BOOK 2: In the context of *matrices*, a particular scalar  $\lambda$  is an eigenvalue of an  $n \times n$  *square matrix*  $A$  if it permits a solution  $X$  to be found to the *matrix eigenvalue equation*

$$AX = \lambda X,$$

where  $X$  is a non-zero  $n \times 1$  *column matrix*.

A similar definition applies to *abstract vectors*: a particular scalar  $\lambda$  is an eigenvalue of an operator  $\hat{A}$  if it permits a solution  $|\psi\rangle$  to be found to the eigenvalue equation

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle,$$

where  $|\psi\rangle$  is a non-zero *vector*.

Strictly speaking, the general rule identifying the eigenvalues of operators with the possible results of measurements applies only if the possible results are discrete. More generally, a modified version of the rule applies, with eigenvalues replaced by *generalized eigenvalues*.

**eigenvalue equation** (B1: 43, 221) In the context of *operators* acting on functions of a single variable, an eigenvalue equation is an equation of the form

$$\hat{A}f(x) = \lambda f(x),$$

where  $\hat{A}$  is an operator acting on the function  $f(x)$  and the *scalar*  $\lambda$  is an undetermined parameter.

Solving the eigenvalue equation involves finding suitable values of  $\lambda$  and the corresponding functions  $f(x)$  that satisfy this equation subject to appropriate

*boundary conditions* (e.g.  $f(x)$  remaining finite as  $x$  tends to  $\pm\infty$ ). The suitable values of  $\lambda$  are the *eigenvalues*, and the corresponding functions are the *eigenfunctions*, of the operator  $\hat{A}$ . The prefix 'eigen' comes from the German for characteristic and indicates the 'special' nature of the eigenfunctions and eigenvalues of an operator.

BOOK 2: A *matrix eigenvalue equation* takes the form

$$AX = \lambda X,$$

where  $X$  is a non-zero *column matrix*.

For *abstract vectors* an eigenvalue equation is written as

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle,$$

where  $|\psi\rangle$  is a non-zero *vector*.

**eigenvector** (B2: 25, 224) In *Dirac notation*, a non-zero *vector*  $|a\rangle$  is said to be an eigenvector of the operator  $\hat{A}$  if

$$\hat{A}|a\rangle = \lambda|a\rangle,$$

where the *scalar* quantity  $\lambda$  is the *eigenvalue* corresponding to  $|a\rangle$ .

An eigenvector of a given *square matrix* is any non-zero *column matrix* that satisfies the *matrix eigenvalue equation* for that matrix.

**Einstein A-coefficient** (B3: 216) A coefficient  $A_{21}$  that characterizes the rate of *spontaneous emission* when a *system* makes a *radiative transition* from one *quantum state* to another. For a large collection of *atoms*, the rate at which atoms make spontaneous transitions from state 2, of energy  $E_2$ , to state 1, of energy  $E_1$ , is

$$\left(\frac{dN_2}{dt}\right)_{\text{spon}} = -A_{21}N_2,$$

where  $N_2$  is the number of atoms in state 2 and  $E_2 > E_1$ .

The Einstein A-coefficient cannot be calculated directly in *quantum mechanics*, but it can be expressed in terms of the *Einstein B-coefficient* which can be calculated using *time-dependent perturbation theory*. Sometimes called the *A-coefficient*.

**Einstein B-coefficient** (B3: 216) A coefficient  $B_{21}$  that characterizes the rate of *stimulated emission* when a *system* makes a *radiative transition* from one *quantum state* to another. For a large collection of *atoms*, the rate at which atoms in state 2 of energy  $E_2$  make stimulated transitions to state 1 of energy  $E_1 < E_2$  is

$$\left(\frac{dN_2}{dt}\right)_{\text{stim}} = -B_{21}N_2u(\omega_{21}),$$

where  $N_2$  is the number of atoms in state 2 and  $u(\omega_{21})$  is the *spectral energy density function* of *electromagnetic radiation* at the *angular frequency*  $\omega_{21} = (E_2 - E_1)/\hbar$ .

Another Einstein  $B$ -coefficient characterizes the process of *absorption*. In this case, the rate at which atoms in state 1 of energy  $E_1$  absorb radiation and make transitions to state 2 of energy  $E_2 > E_1$ , is

$$\left(\frac{dN_1}{dt}\right)_{\text{abs}} = -B_{12}N_1u(\omega_{21}),$$

where  $N_1$  is the number of atoms in state 1.

It turns out that  $B_{21} = B_{12}$ . Both  $B_{21}$  and  $B_{12}$  are called Einstein  $B$ -coefficients, and they can be calculated using *time-dependent perturbation theory*. Sometimes called the  $B$ -coefficient. Compare with the *Einstein A-coefficient*.

**elastic scattering** (B1: 196) *Scattering* in which *kinetic energy* is conserved and *particles* do not change their nature or their *quantum state* of internal excitation; nor are they created, destroyed or absorbed. Contrast with *inelastic scattering*.

**electric charge** A fundamental property of matter that determines the *electric* and *magnetic forces* between *particles*. There are two types of charge: positive and negative. *Protons* are positively charged (with charge  $e$ ) and *electrons* are negatively charged (with charge  $-e$ ). The *SI* unit of charge is the coulomb (C) and  $e = 1.60 \times 10^{-19}$  C.

**electric current** The electric current along a wire is the rate of flow of *electric charge* through a fixed plane perpendicular to the axis of the wire. If the current is carried by *electrons* (which are negatively-charged), it is in the opposite direction to the direction of flow of electrons.

**electric dipole approximation** (B3: 201) An approximation that represents the interaction between an *atom* and an *electromagnetic wave* by the time-dependent *potential energy function*

$$V(t) = e \sum_i \mathcal{E}(t) \cdot \mathbf{r}_i,$$

where  $\mathcal{E}(t)$  is the *electric field* at time  $t$  due to the electromagnetic wave at the position of the atom (assumed uniform throughout the atom),  $\mathbf{r}_i$  is the position of the  $i$ th *electron*,  $e$  is the *magnitude* of the electron *charge* and the sum is over all the electrons in the atom.

**electric dipole moment** (B3: 201) The electric dipole moment of a collection of charged *particles*  $q_i$  at positions  $\mathbf{r}_i$  is given by  $\sum_i q_i \mathbf{r}_i$ . With the origin fixed at the *nucleus*, the electric dipole moment of an *atom* is  $-e \sum_i \mathbf{r}_i$ , where  $\mathbf{r}_i$  is the position of the  $i$ th *electron*.

**electric field** A *vector* field that determines the *electric force* on a charged *particle* placed at any given point. The electric field at point P is the electric force per unit *charge* experienced by a small test charge placed at P. The *SI* unit of electric field is  $\text{N C}^{-1}$ .

**electric force** The force experienced by a charged *particle* due to an *electric field*, given by

$$\mathbf{F} = q\mathcal{E},$$

where  $q$  is the *charge* of the particle and  $\mathcal{E}$  is the electric field at the position of the particle.

**electrical conductivity** (B3: 188) A measure of the ease with which a material conducts an *electric current*. If a homogeneous slab of material of length  $l$  and cross-sectional area  $A$  has a potential difference  $V$  maintained across its ends, the current flowing through the slab has *magnitude*

$$i = \frac{\sigma AV}{l},$$

where  $\sigma$  is the electrical conductivity of the material. A wire of length  $l$  and cross-sectional area  $A$  has electrical resistance  $R = l/A\sigma$ . The *SI* unit of electrical conductivity is  $\text{ohm}^{-1}\text{metre}^{-1} = \Omega^{-1}\text{m}^{-1}$ .

**electromagnetic radiation** Self-sustaining electromagnetic disturbances that propagate through space with *electric* and *magnetic fields* decreasing no faster than  $1/\text{distance}$ , and the corresponding *energy density* decreasing no faster than  $1/\text{distance}^2$ . Realized through *electromagnetic waves*.

**electromagnetic wave** A *transverse wave* in which an *electric field* and a *magnetic field* oscillate *in phase* with one another. The simplest type of electromagnetic wave is a *monochromatic plane wave* in a homogeneous medium; such a wave is *sinusoidal*, with a constant values of *frequency*  $f$ , *wavelength*  $\lambda$  and speed  $f\lambda$ . In a vacuum, the speed of all electromagnetic waves is a universal constant, the *speed of light*  $c$ . See also *electromagnetic radiation*.

**electron** A negatively-charged *particle*, currently regarded as structureless, with about one two-thousandth the mass of a *proton*. Electrons are the carriers of *electric current* in metallic *conductors*.

BOOK 2: Electrons are *spin- $\frac{1}{2}$  particles*, and hence are *fermions* which obey the *Pauli exclusion principle*.

**electronic configuration** (B3: 126, 161) For an *atom* described in the *central-field approximation*, the electronic configuration is a list showing the numbers of *electrons* in occupied *shells*. The list is written in *spectroscopic notation*, with the number of electrons in each shell indicated by a superscript. For example, the *ground-state* electronic configuration of carbon is  $1s^2 2s^2 2p^2$ .

For a *molecule* described in the *LCAO approximation*, the electronic configuration is a list showing the numbers of electrons in the different types of occupied *molecular orbital*. The list is written in spectroscopic notation, with the number of electrons in each type of molecular orbital indicated by a superscript. For example, the ground-state electronic configuration of diatomic lithium is  $1\sigma_g^2 1\sigma_u^2 2\sigma_g^2$ .

The abbreviation *configuration* is sometimes used.

**electronic energy** (B3: 144) In the *Born–Oppenheimer approximation*, the electronic energy is an *eigenvalue* of the *electronic time-independent Schrödinger equation*. For a given *electronic state* in a *diatomic molecule*, it gives the total *energy* of the *electrons* for a particular internuclear separation. The electronic energy also contributes to the *total static energy*, which appears in the *nuclear time-independent Schrödinger equation* and provides the effective *potential energy function* in which the *nuclei* move.

**electronic energy eigenfunction** (B3: 144) A function of the positions of the *electrons* in a *molecule*, which is a solution of the *electronic time-independent Schrödinger equation* for the molecule for a set of fixed nuclear positions.

**electronic time-independent Schrödinger equation** (B3: 144) A *time-independent Schrödinger equation* that describes the behaviour of the *electrons* in a *molecule* in the *Born–Oppenheimer approximation*. The equation neglects the *kinetic energies* and the mutual *potential energy* of the *nuclei*. It provides a set of *electronic energies* and *electronic energy eigenfunctions* for fixed nuclear positions.

**electronvolt** (B1: 11) A unit of *energy* defined as the *magnitude* of the energy gained when an *electron* is accelerated through a potential difference of one volt. An electronvolt is given the symbol eV, and is equal to  $1.60 \times 10^{-19}$  J.

According to the conventional rules for *SI* prefixes,  $1 \text{ meV} = 10^{-3} \text{ eV}$ ,  $1 \text{ keV} = 10^3 \text{ eV}$ ,  $1 \text{ MeV} = 10^6 \text{ eV}$  and  $1 \text{ GeV} = 10^9 \text{ eV}$ . The units meV, eV, MeV and GeV are convenient for discussing molecular rotations, electronic transitions, nuclear physics and *elementary particle* physics, respectively.

**electrostatic force** The force between stationary charged *particles*. For two particles in a vacuum, this force is given by *Coulomb's law*.

**electrostatic potential energy** *Potential energy* due to *electrostatic forces*. For two *particles* in a vacuum, the electrostatic potential energy is given by the *Coulomb potential energy function*.

**element** (i) An abbreviation for *chemical element*. Traditionally, an element is a substance that cannot be divided by chemical means, heating or the passage of an *electric current*. More precisely, a sample of any given element consists of matter entirely composed of *atoms* with the same *atomic number*, and hence the same number of *protons* in their *nuclei*.

(ii) In mathematics, an element is a basic part of something (e.g. a volume element or a *matrix element*).

**elementary particle** A piece of matter that is

smaller than a *nucleus*. Such *particles* include *protons* and *neutrons*, as well as *electrons* and *quarks*. They may or may not be truly fundamental constituents of matter.

**emission** See *spontaneous emission* and *stimulated emission*.

**energy** In *classical physics*, energy is the property of a *system* that measures its capacity for doing work on a body, or for changing the *kinetic energy* of a *free particle*. Energy is a *scalar* quantity that is conserved in any *isolated system*. The *SI* unit of energy is the joule, represented by the symbol J, where  $1 \text{ J} = 1 \text{ N m} = 1 \text{ kg m}^2 \text{ s}^{-2}$ .

**energy band** (B3: 174) A set of *energy levels* for *electrons* in a solid that are extremely closely spaced within a finite range of *energies* and may be separated from other energy bands by *band gaps*.

**energy curve** (B3: 154) A plot of the *total static energy* of a *diatomic molecule* as a function of the internuclear distance *R*.

**energy density** For *electromagnetic radiation*, the energy density at a given point is the *energy* per unit volume in a small volume element around the point. For an *electromagnetic wave* in a vacuum with an *electric field* of amplitude  $\mathcal{E}_0$ , the time-averaged energy density is  $\frac{1}{2}\epsilon_0\mathcal{E}_0^2$ , where  $\epsilon_0$  is the *permittivity of free space*.

**energy eigenfunction** (B1: 56) An *eigenfunction* of the *Hamiltonian operator* for a given *system*, and therefore a solution of the *time-independent Schrödinger equation* for the system. If the *quantum state* of a system is described by a particular energy eigenfunction, any *measurement* of the *energy* of the system is certain to give the corresponding *energy eigenvalue*.

**energy eigenvalue** (B1: 56) An *eigenvalue* of the *Hamiltonian operator* for a given *system*. Each energy eigenvalue is an allowed *energy* of the system.

**energy level** (B1: 10) An *energy* that characterizes a particular *quantum state* of a *system*. In *bound systems*, such as *nuclei*, *atoms* and *molecules*, the energy levels are discrete. When such systems become unbound, as in the case of an *ionized atom*, the energy levels form a *continuum*. Do not confuse energy levels with quantum states: if an energy level is *degenerate* it corresponds to more than one quantum state.

**energy quantization** (B1: 70) The quantum phenomenon in which *bound states* have discrete *energy levels*.

**entangled state** (B2: 150) A *wave function* or *state vector* describing the *state* of a many-particle *system* represents an entangled state if it cannot be expressed as a product of terms each specifying the state of a single *particle*. *Entanglement* does not depend upon



the *basis* used to describe the state. If a system is in an entangled state, its individual particles do not have their own states, although the system as a whole does.

**entanglement** (B2: 149) *Particles in an entangled state* are said to be in a state of entanglement.

**EPR argument** (B2: 157) An argument that highlights the uncomfortable fact that *quantum mechanics* predicts non-local correlations for *measurements* on pairs of separated *particles* in an *entangled state*. For example, in a *Bohm-type experiment* on *spin- $\frac{1}{2}$  particles* in a *singlet state*, quantum mechanics predicts that measurements of the *spin components* of the two particles will always give opposite results along any given axis. Making assumptions of *locality* and *realism*, the EPR argument maintains that, prior to any measurement, this implies that each particle must actually have definite values of spin (determined by *local hidden variables*) along all possible axes. Since this is contrary to the quantum-mechanical view (and is specifically contrary to the *generalized uncertainty principle*), Einstein asserted that quantum mechanics must be incomplete.

The EPR argument backfires. *Bell's theorem* shows that *local hidden-variable theories* cannot reproduce all the predictions of quantum mechanics, and actual experiments give results that violate *Bell's inequalities*; such results cannot be explained by local hidden-variable theories, but can be explained by quantum mechanics.

**equation of continuity** (B1: 189) An equation used in the description of fluid flow that relates changes in the density of fluid in any small region to currents carrying fluid through the boundaries of that region. In *wave mechanics*, the *probability density* and *probability current* obey a similar equation of continuity.

**equilibrium separation** (B3: 154) The value of the distance between the *nuclei* of a *diatomic molecule* at which the *energy curve* reaches its lowest point and the *total static energy* has its minimum value.

**equivalent electrons** (B3: 136) *Electrons* belonging to the same *shell* (that is, having the same *n* and *l* quantum numbers). The possible *atomic terms* of a pair of equivalent electrons are restricted by the *Pauli exclusion principle* and by the fact that the electrons are *indistinguishable particles*. Contrast with *non-equivalent electrons*.

**Euler's formula** (B1: 214) The relationship

$$e^{i\theta} = \cos \theta + i \sin \theta$$

that links the exponential function to the cosine and sine functions.

**even function** (B1: 78) A function  $f(x)$  for which  $f(-x) = f(x)$  for all  $x$ . Contrast with *odd function*.

**even parity** (B3: 22) A function is said to have even parity if it remains unchanged under the operation of *inversion*. Equivalently, it is said to have *parity* +1. Compare with *even function*. Contrast with *odd parity*.

**exchange** (B3: 123) A purely quantum-mechanical effect that modifies the *energy* of a *system* of *electrons* and arises because the electrons are *indistinguishable fermions*.

**exchange integral** (B3: 122) An integral of the form

$$J_{rs} = \frac{e^2}{4\pi\epsilon_0} \iint \frac{\phi_r^*(\mathbf{r}_1) \phi_s^*(\mathbf{r}_2) \phi_s(\mathbf{r}_1) \phi_r(\mathbf{r}_2)}{r_{12}} dV_1 dV_2$$

that partly describes the average *Coulomb potential energy* of two *electrons* occupying *orbitals*  $\phi_r$  and  $\phi_s$  in an *atom* or *molecule*.

The exchange integral is a quantum-mechanical *interference* term arising from the fact that the two electrons are *indistinguishable*. The exchange integral must be added to or subtracted from the *Coulomb integral*, depending on whether the *spatial wave function* describing the pair of electrons is *symmetric* or *antisymmetric*. This quantifies the quantum-mechanical phenomenon of *exchange*.

**excited state** A *quantum state* of a given *system* with an *energy* that is greater than the *ground-state energy* of the system.

**exciton** (B3: 190) A *hydrogen-like system* formed when an *electron* in the *conduction band* and a *hole* in the *valence band* of a *semiconductor* form a *bound state* through mutual electrostatic attraction. The *binding energy* is very small, so excitons are observed only at low temperatures.

**expectation value** (B1: 111, 229) For a given *random variable*  $A$ , the expectation value  $\langle A \rangle$  is the theoretical prediction for the *average value* of  $A$  in the limiting case of a large number of *measurements*.

Given a discrete set of possible outcomes,  $A_1, A_2, \dots$ , with *probabilities*  $p_1, p_2, \dots$ , the expectation value of  $A$  is given by

$$\langle A \rangle = \sum_i p_i A_i,$$

where the sum runs over all the possible values for  $A$ .

For a random variable  $x$  with a continuous set of possible outcomes, the expectation value is given by

$$\langle x \rangle = \int_{-\infty}^{\infty} \rho(x) x dx,$$

where  $\rho(x)$  is the *probability density function* for  $x$ .

In *quantum mechanics*, the expectation value of an *observable*  $A$  is the quantum-mechanical prediction for the average value of  $A$  when measurements are taken on a large number of identical *systems* all prepared in the same *quantum state*. In

one-dimensional *wave mechanics*, the expectation value of  $A$  is given by the *sandwich integral rule*

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{A} \Psi(x, t) dx,$$

where  $\hat{A}$  is the quantum-mechanical *operator* representing the observable  $A$  and  $\Psi(x, t)$  is the *wave function* of the system at the instant of measurement.

BOOK 2: In *Dirac notation*, the expectation value of  $A$  is given by the *sandwich rule*

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle,$$

where  $|\Psi\rangle$  is the *state vector* of the system at the instant of measurement.

**expectation value for spin** (B2: 88) If a *spin- $\frac{1}{2}$  particle* is in a *spin state*  $|\uparrow_n\rangle$  that is certain to give the value  $+\hbar/2$  for the *spin component* in the  $n$ -direction, the *expectation value* of any specified spin component (say  $S_x$ ) in this state is

$$\langle S_x \rangle = p_u \left( \frac{\hbar}{2} \right) + p_d \left( -\frac{\hbar}{2} \right)$$

where  $p_u = |\langle \uparrow_x | \uparrow_n \rangle|^2$  is the *probability* of getting the value  $+\hbar/2$  when spin is measured in the  $x$ -direction and  $p_d = |\langle \downarrow_x | \uparrow_n \rangle|^2$  is the probability of getting the value  $-\hbar/2$  when spin is measured in the  $x$ -direction.

Alternatively, we can use the *sandwich rule for spin* to write

$$\langle S_x \rangle = \langle \uparrow_n | \hat{S}_x | \uparrow_n \rangle,$$

where  $\hat{S}_x$  is the *spin angular momentum operator* for the  $x$ -component of spin. This is generally represented by a  $2 \times 2$  *square matrix*, while  $|\uparrow_n\rangle$  is represented by a *column matrix* and  $\langle \uparrow_n |$  is represented by a *row matrix*.

**exponential form** (B1: 214) A *complex number* is said to be expressed in exponential form if it is written as

$$z = re^{i\theta},$$

where the *real numbers*  $r \geq 0$  and  $\theta$  are called respectively the *modulus* and *phase* of the complex number. Any complex number can be expressed in this form. See also *Cartesian form* and *polar form*.

**exponential law of radioactive decay** (B1: 13) The physical law stating that, given a large sample of *nuclei* of a given type, the average number of nuclei that remain undecayed at time  $t$  falls exponentially as

$$N(t) = N(0) e^{-\lambda t},$$

where  $N(0)$  is the initial number of nuclei at time  $t = 0$  and  $\lambda$  is the *decay constant* for the given type of nucleus.

**F-centre** (B1: 83) A defect in an *ionic crystal* (such as NaCl) in which an ejected negative *ion* is replaced by an *electron* that acts as a *particle* trapped in a three-dimensional box created by the surrounding ions. F-centres can absorb one or more *wavelengths* of *visible light* when the trapped electron makes an upward transition between discrete *energy levels*; if present in sufficient numbers, F-centres can alter the colour of a crystal.

**Fermi energy** (B3: 185) An energy  $E_F$  that characterizes the occupation of the *states* of *electrons* in a given material. At *absolute zero*, all electron states with *energies* less than  $E_F$  are full, while all electron states with energies greater than  $E_F$  are empty. In a *conductor* at absolute zero, the Fermi energy is the energy of the highest occupied electron state. In a *semiconductor* or *insulator*, at absolute zero, the Fermi energy is conventionally placed in the *band gap* between the *valence band* and the *conduction band*; in the absence of impurities, it is in the middle of the band gap.

**fermion** (B2: 116) A *particle* whose *spin quantum number* is a half-integer:  $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ . Examples include *electrons*, *protons*, *neutrons* and *quarks*. A composite particle containing an odd number of fermions is a fermion. A system of *identical* fermions is described by an *antisymmetric total wave function* and obeys the *Pauli exclusion principle*. Contrast with *boson*.

**fine structure** (B3: 90) The splitting of *spectral lines* that becomes evident with high-resolution measurements. In *atoms*, fine structure is due to a breaking of the *degeneracy* of *quantum states* by:

- relativistic contributions to the *kinetic energy*;
- *spin-orbit interactions*;
- the *Darwin term*.

The spacing between *energy levels* in the fine structure of the *hydrogen atom spectrum* is typically a factor of  $\alpha^2$  smaller than the spacing between energy levels in the gross structure predicted by the *Coulomb model*, where  $\alpha$  is the *fine structure constant*.

**fine structure constant** (B3: 104) A dimensionless constant (i.e. one that is equal to a pure number, independent of the system of units) which sets the scale of *fine structure* splitting in *atoms*, and is given by the expression

$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} = (137.035\,999\,679 \pm 0.000\,000\,094)^{-1},$$

where  $e$  is the *magnitude* of the *charge* of an *electron*,  $\epsilon_0$  is the *permittivity of free space*,  $\hbar$  is *Planck's constant* divided by  $2\pi$  and  $c$  is the *speed of light* in a vacuum.

The ratio of the speed of an electron in the lowest orbit of the *Bohr model* of hydrogen to the *speed*

*of light* in a vacuum is equal to  $\alpha$ , and the most important relativistic corrections to the *energy levels* of a *hydrogen atom* are of order  $\alpha^2$ .

**finite barrier** Any member of a class of *potential energy functions* that are finite everywhere, possess a local maximum, and approach a lower constant value (usually taken to be zero) at large distances from the maximum.

**finite square barrier** (B1: 181) In one dimension, a *potential energy function* characterized by a constant value of *potential energy* (usually positive) over a finite continuous region of space, with a smaller constant value (usually zero) elsewhere.

The concept can be generalized to two and three dimensions. In this case, the squareness of barrier describes the abruptness of the change in potential energy; a square barrier may occupy any region in space (e.g. a cube or a sphere in three dimensions).

**finite square step** (B1: 184) In one dimension, a *potential energy function* characterized by a constant value of *potential energy* over some semi-infinite region of space, with a different constant potential energy elsewhere.

**finite square well** (B1: 85) In one dimension, a *potential energy function* characterized by a constant value of *potential energy* (usually negative) over a finite continuous region of space, with a larger constant value (usually zero) elsewhere. Such a well has a finite number of *bound states* ( $\geq 1$ ).

The concept can be generalized to two and three dimensions. In this case, the squareness of well describes the abruptness of the change in potential energy; a square well may occupy any region in space (e.g. a cube or a sphere in three dimensions).

**finite well** (B1: 56) Any member of a class of *potential energy functions* that are finite everywhere, possess a local minimum, and approach a higher constant value (usually taken to be zero) at large distances from the minimum.

**first ionization energy** (B3: 130) The *energy* required to remove a single *electron* from a neutral *atom* or *molecule*.

**first-order approximation** (B3: 80) See *order of approximation*.

**first-order correction** In *perturbation theory*, the first-order correction is the additional term, proportional to the *perturbation*, that must be added to the *zeroth-order approximation* to produce the *first-order approximation*.

**first-order partial derivative** (B1: 224) A function obtained by taking the *partial derivative* of a given function. Given a function  $f(x, y)$  of two variables, we can define two first-order partial derivatives:  $\partial f / \partial x$  is the rate of change of  $f$  with respect to  $x$

when  $y$  is held constant, and  $\partial f / \partial y$  is the rate of change of  $f$  with respect to  $y$  when  $x$  is held constant.

**first-order perturbation theory** (B3: 83, 205)

An approximation method that includes constant terms and terms proportional to the first power of a small *perturbation*, but systematically neglects terms involving the second and higher powers of the perturbation. It may refer either to *time-independent perturbation theory* or to *time-dependent perturbation theory*.

**flux** (B1: 196) A quantity that describes the rate of flow of *particles* around a given point in three-dimensional space. The flux is the rate of flow of particles, per unit time per unit area, through a tiny area centred on the given point and perpendicular to the direction of flow of particles at the point. The *SI* unit of flux is  $\text{m}^{-2} \text{s}^{-1}$ . Compare with *beam intensity*.

**forbidden transition** (B3: 209) A *radiative transition* that is forbidden according to the *electric dipole approximation* and first-order *time-dependent perturbation theory*. Such a transition fails to satisfy corresponding *selection rules*.

**force constant** (B1: 125) The positive constant  $C$  that appears in *Hooke's law*,  $F_x = -Cx$ , and in the expression for the *potential energy function* of a *simple harmonic oscillator*,  $V(x) = \frac{1}{2}Cx^2$ . The *SI* unit of a force constant is  $\text{N m}^{-1}$ .

**formal bond order** (B3: 163) In the *LCAO approximation*, the formal bond order of a *diatomic molecule* is given by  $(n_b - n_a)/2$ , where  $n_b$  is the number of *electrons* in *bonding orbitals* and  $n_a$  is the number of electrons in *antibonding orbitals*. Often abbreviated to *bond order*.

**Fourier transform** (B1: 171) The Fourier transform  $A(k)$  of a function  $f(x)$  is defined by

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx.$$

In one dimension, the *momentum amplitude*  $A(k)$  of a *free particle* is the Fourier transform of the initial *wave function*,  $\Psi(x, 0)$ . More generally, the momentum amplitude  $A(k, t)$  of any *particle* at time  $t$  can be taken to be the Fourier transform of the wave function,  $\Psi(x, t)$ . See also *inverse Fourier transform*. BOOK 3: See also the *three-dimensional Fourier transform*.

**frame of reference** A set of coordinate axes and synchronized clocks, which makes it possible to specify uniquely the location in space and time of any given event.

**free particle** (B1: 166) A *particle* that is subject to no forces, and for which the *potential energy* is a constant independent of position (usually set equal to zero).



**frequency** (B1: 10, 17) The number of *cycles* per unit time of an *oscillation* or *wave*. The frequency  $f$  is related to the *period*  $T$  by  $f = 1/T$ . The *SI* unit of frequency is the *hertz* ( $1 \text{ Hz} = 1 \text{ s}^{-1}$ ). Compare with *angular frequency*.

**function space** (B2: 13) A *vector space* that represents all *normalizable functions*, and is used to express the results of *wave mechanics* in compact *Dirac notation*. For further interest see *Hilbert space*.

**fusion** (B1: 205) An abbreviation for *nuclear fusion*.

**Gaussian function** (B1: 131) A function of the form

$$f(x) = C_0 e^{-x^2/2a^2},$$

where  $C_0$  and  $a$  are constants. The *energy eigenfunctions* of a *harmonic oscillator* all involve Gaussian functions.

**Gaussian wave packet** (B1: 182) A *wave packet* for which the square of the *modulus* of the *wave function*,  $|\Psi|^2$ , is shaped like a *Gaussian function* (for a suitable choice of origin).

**Geiger counter** A device for detecting *particles* that are able to cause the *ionization* of *molecules* in a gas. Also called a Geiger–Müller tube.

**Geiger–Nuttall relation** (B1: 203) A relation linking the *decay constant*  $\lambda$  of a *nucleus* that emits *alpha particles* to the *alpha-particle emission energy*  $E_\alpha$  of that nucleus. The relation applies to specific families of nuclei (such as *isotopes* of a given nucleus) and may be written in the form

$$\lambda = Ae^{-B/E_\alpha^{1/2}},$$

where  $A$  is a constant that characterizes the particular family of nuclei, and  $B$  depends on the *charge* of the individual nucleus.

**general solution** (B1: 218) For *differential equations*, the general solution is an expression that describes the general family of functions that satisfy the differential equation. If the *order of a differential equation* is  $n$ , the general solution of the equation contains  $n$  *arbitrary constants*.

**general spin matrix** (B2: 82) The  $2 \times 2$  *Hermitian matrix* that serves as the quantum-mechanical *operator* representing the *spin component* of a *spin- $\frac{1}{2}$  particle* in an arbitrary direction.

If the spin component is measured in the direction of the *unit vector*  $\mathbf{n} = \sin \theta \cos \phi \mathbf{e}_x + \sin \theta \sin \phi \mathbf{e}_y + \cos \theta \mathbf{e}_z$ , where  $\theta$  and  $\phi$  are the *polar angle* and the *azimuthal angle* of *spherical coordinates*, the general spin matrix is

$$\hat{S}_{\mathbf{n}} = \frac{\hbar}{2} \begin{bmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & -\cos \theta \end{bmatrix},$$

where  $\hbar$  is *Planck's constant* divided by  $2\pi$ . This matrix has *eigenvectors*

$$|\uparrow_{\mathbf{n}}\rangle = \begin{bmatrix} \cos(\theta/2) \\ e^{i\phi} \sin(\theta/2) \end{bmatrix}$$

and

$$|\downarrow_{\mathbf{n}}\rangle = \begin{bmatrix} -e^{-i\phi} \sin(\theta/2) \\ \cos(\theta/2) \end{bmatrix}$$

with *eigenvalues*  $+\hbar/2$  and  $-\hbar/2$ , respectively.

**generalized Ehrenfest theorem** (B2: 30) The statement that

$$\frac{d\langle A \rangle}{dt} = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle,$$

where  $d\langle A \rangle/dt$  is the rate of change of the *expectation value* of  $A$  in a given *quantum state* in an *isolated system*,  $\hat{H}$  is the *Hamiltonian operator* of the system, and the expectation values on both sides of the equation refer to the given state.

The generalized Ehrenfest theorem assumes that the Hamiltonian operator does not depend explicitly on time. It implies that the expectation value of a quantity  $A$  remains constant in time if the corresponding operator  $\hat{A}$  *commutes* with the Hamiltonian operator (in which case,  $A$  is called a *conserved quantity*). See also *Ehrenfest's theorem*, which covers the special cases  $\hat{A} = \hat{x}$  and  $\hat{A} = \hat{p}_x$ .

**generalized eigenvalue** (B2: 142) A generalization of the concept of an *eigenvalue*. For an *operator*  $\hat{A}$  and a fixed *scalar*  $\lambda$ , we construct the equation

$$(\hat{A} - \lambda \hat{I})|f\rangle = |\eta\rangle,$$

where  $\hat{I}$  is the *identity operator*. We then say that  $\lambda$  is a generalized eigenvalue of  $\hat{A}$ , if  $\langle \eta|\eta \rangle$  can be made arbitrarily small by a suitable choice of  $|f\rangle$ .

The allowed values of any *observable* are given by the generalized eigenvalues of the corresponding quantum-mechanical operator (even if these form a *continuum*). In cases where the allowed values form a discrete set, the eigenvalues of the quantum-mechanical operator are themselves generalized eigenvalues.

**generalized uncertainty principle** (B2: 35) This principle states that

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [\hat{A}, \hat{B}] \rangle \right|,$$

where  $\Delta A$  and  $\Delta B$  are the *uncertainties* of *observables*  $A$  and  $B$  in a given *quantum state*, and the right-hand side involves the *expectation value* of the *commutator* of the operators  $\hat{A}$  and  $\hat{B}$  in the same state. The generalized uncertainty principle reduces to the *Heisenberg uncertainty principle* in the special case  $\hat{A} = \hat{x}$  and  $\hat{B} = \hat{p}_x$ .

**gerade orbital** (B3: 158) A *molecular orbital* in a *diatomic molecule* that has *even parity* under the operation of *inversion* about the *centre of symmetry* of the molecule. The word ‘gerade’ means ‘even’

in German. Gerade orbitals are indicated by the subscript g. Contrast with *ungerade*.

**GHZ state** (B2: 169) An *entangled state* of three *particles* used to test for the existence of *local hidden variables*. For *spin- $\frac{1}{2}$  particles*, this state takes the form

$$\frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\rangle - |\downarrow\downarrow\downarrow\rangle).$$

For *linearly-polarized photons*, it takes the form

$$\frac{1}{\sqrt{2}}(|V V V\rangle + |H H H\rangle).$$

GHZ states are used in tests of *local hidden-variable theories*, and have the advantage of not relying on the averaging of experimental results.

**good quantum number** (B3: 28, 133) A *quantum number* labelling the *eigenfunctions* of an operator that commutes with the *Hamiltonian operator* of a given system. Each *energy eigenfunction* is generally labelled by a set of good quantum numbers, which characterize the values of a set of *compatible observables*, including *energy*.

**ground state** (B1: 10) The *quantum state* of lowest *energy* in a given system. In the case of a system that displays *degeneracy*, there may be more than one such state. Contrast with *excited state*.

**group** (B3: 128) The set of *elements* in a single column of the *Periodic Table*. Elements from a group have similar *spectra* and a similar chemistry, tending to form similar types of *molecule* when combining with other *atoms*. Contrast with *period*.

**gyromagnetic ratio** (B2: 45, 90) For a system with *orbital angular momentum* and no *spin*, the gyromagnetic ratio is the proportionality constant  $\gamma$  in the equation  $\boldsymbol{\mu} = \gamma \mathbf{L}$  that links the *magnetic dipole moment*  $\boldsymbol{\mu}$  to the orbital angular momentum,  $\mathbf{L}$ .

For a system with spin and no orbital angular momentum, the gyromagnetic ratio is called the *spin gyromagnetic ratio*. This is the proportionality constant  $\gamma_s$  in the equation  $\boldsymbol{\mu} = \gamma_s \mathbf{S}$  linking the magnetic dipole moment  $\boldsymbol{\mu}$  to the *spin angular momentum*,  $\mathbf{S}$ .

**half-life** (B1: 14) For a given type of unstable *nucleus* or unstable *particle*, the time over which half the nuclei or particles, on average, decay. The half-life  $T_{1/2}$  is related to the *decay constant*  $\lambda$  by  $T_{1/2} = \ln 2 / \lambda$ .

**half-silvered mirror** (B1: 15) A mirror coated in such a way that if many *photons* fall on any part of it, at an angle of incidence of  $45^\circ$ , half are transmitted and half are reflected. A single photon incident on a half-silvered mirror emerges in a *linear superposition* of two *states* corresponding to transmission and reflection, and the *probability amplitudes* for these

states have equal *magnitudes*. A half-silvered mirror is an example of a *beam splitter*.

**halogen atoms** (B3: 129) *Chemical elements* in the penultimate group of the *Periodic Table*, namely fluorine (F), chlorine (Cl), bromine (Br), iodine (I) and astatine (At). Halogen atoms lack a single *electron* in an open *p-shell*. They react strongly with *alkali atoms*.

**Hamiltonian** (B3: 67) In *quantum mechanics*, the term ‘Hamiltonian’ is sometimes used as an abbreviation for the *Hamiltonian operator*.

**Hamiltonian function** (B1: 47) A function which, in *classical mechanics*, expresses the total *energy* of a system as a sum of (i) the *kinetic energy* expressed in terms of *momentum*, and (ii) the *potential energy function* of the system.

**Hamiltonian matrix** (B2: 91) For a *spin- $\frac{1}{2}$  particle* in a *magnetic field*, the Hamiltonian matrix is a  $2 \times 2$  matrix that provides the *Hamiltonian operator* in *spin space*. It takes the form

$$\hat{H} = -\gamma_s B \hat{S}_n = -\frac{\gamma_s B \hbar}{2} \begin{bmatrix} \cos \theta & e^{-i\phi} \sin \theta \\ e^{i\phi} \sin \theta & -\cos \theta \end{bmatrix},$$

where  $\gamma_s$  is the *spin gyromagnetic ratio*,  $B$  is the *magnitude* of the magnetic field,  $\hat{S}_n$  is the *general spin matrix*,  $\hbar$  is *Planck’s constant* divided by  $2\pi$ , and  $\theta$  and  $\phi$  are the *polar* and *azimuthal angles* of *spherical coordinates*.

**Hamiltonian operator** (B1: 48) The quantum-mechanical *operator* corresponding to the total *energy* of a system, obtained from the classical *Hamiltonian function* of the system by replacing each *observable* quantity by the corresponding quantum-mechanical operator.

The Hamiltonian operator appears in *Schrödinger’s equation*, the *time-independent Schrödinger equation* and in quantum mechanical expressions for the *expectation value* and *uncertainty* of the energy. BOOK 2: It also appears in the *generalized Ehrenfest theorem*.

The abbreviated term *Hamiltonian* is sometimes used.

**harmonic oscillator** (B1: 124) A system described by a classical *Hamiltonian function* of the form

$$H = \frac{p_x^2}{2m} + \frac{1}{2} C x^2 = \frac{p_x^2}{2m} + \frac{1}{2} m \omega_0^2 x^2,$$

where  $m$  is the mass of the oscillating *particle*,  $x$  is its displacement,  $p_x$  is its *momentum*,  $C$  is the *force constant* and  $\omega_0$  is the *angular frequency*.

In *classical physics*, the *restoring force* on the oscillating particle is proportional to its displacement, and the resulting *simple harmonic motion* is *sinusoidal* in time.

In *wave mechanics*, a harmonic oscillator obeys the *Schrödinger equation*

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + \frac{1}{2} m \omega_0^2 x^2 \Psi(x, t)$$

where  $\omega_0$  is now called the classical angular frequency.

**Heisenberg uncertainty principle** (B1: 117) The principle asserting that, in all *systems* and all *states*, the *uncertainties* of the position and *momentum* components of a *particle* obey the inequality

$$\Delta x \Delta p_x \geq \frac{\hbar}{2},$$

where  $\hbar$  is *Planck's constant* divided by  $2\pi$ .

BOOK 2: This is a special case of the *generalized uncertainty principle*.

**helium atom** An *atom* with *atomic number*  $Z = 2$ , and therefore with two *protons* in its *nucleus*, and two *electrons* outside the nucleus. A helium-4 atom has two *neutrons* in its nucleus (an *alpha particle*) while the rarer *isotope* helium-3 has only one neutron in its nucleus.

**Hermite polynomial** (B1: 134) A polynomial  $H_n(x/a)$  in  $x/a$  that appears in the *energy eigenfunctions* of a *harmonic oscillator*:

$$\psi_n(x) = C_n H_n(x/a) e^{-x^2/2a^2},$$

where  $a$  is the *length parameter* of the oscillator and  $C_n$  is a *normalization constant*.

The  $n$ th-order Hermite polynomial  $H_n(x)$  in  $x$  is defined by

$$H_n(x) = e^{x^2/2} \left( x - \frac{d}{dx} \right)^n e^{-x^2/2} \quad \text{for } n = 0, 1, 2, \dots$$

**Hermitian conjugation** (B2: 219, 221) For a *matrix*  $A$ , the act of transposing the matrix (interchanging its rows and columns), and then taking the *complex conjugate*. Under Hermitian conjugation the *matrix element*  $A_{ij}$  becomes  $A_{ji}^*$ .

**Hermitian matrix** (B2: 81, 221) A *square matrix* that is unchanged by the act of *Hermitian conjugation*. The *matrix elements* of a Hermitian matrix obey the condition  $A_{ij} = A_{ji}^*$ .

Hermitian matrices act as *Hermitian operators* on the *column matrices* that represent *vectors*. This means that their *eigenvalues* are *real*, and *eigenvectors* corresponding to different eigenvalues are *orthogonal*.

**Hermitian operator** (B2: 24, 221) An *operator*  $\hat{A}$  acting on *abstract vectors* in a *vector space* is Hermitian if

$$\langle \hat{A}f | g \rangle = \langle f | \hat{A}g \rangle,$$

for all vectors  $|f\rangle$  and  $|g\rangle$  in the space.

In *function space*, this is interpreted as a relationship between *overlap integrals*:

$$\int_{-\infty}^{\infty} [\hat{A}f(x)]^* g(x) dx = \int_{-\infty}^{\infty} f^*(x) [\hat{A}g(x)] dx$$

for all *normalizable functions*  $f(x)$  and  $g(x)$ .

The *expectation values* and *eigenvalues* of Hermitian operators are *real*. Their *eigenfunctions* (or *eigenvectors*) corresponding to different eigenvalues are *orthogonal*. In *quantum mechanics* all *observables* are represented by *linear Hermitian operators*.

**hertz** The *SI* unit of *frequency*, represented by the symbol Hz. A frequency of 1 Hz is equivalent to one *cycle per second*, so  $1 \text{ Hz} = 1 \text{ s}^{-1}$ .

**hidden variables** (B2: 146) Hypothetical variables that are supposed to determine the results of *measurements* with certainty, but are absent from the quantum-mechanical description. Proponents of *hidden-variable theories* reject the *indeterministic* features of *quantum mechanics* in favour of the doctrine of *realism*. They believe that all *observables* have definite values independent of any act of measurement; these values are supposed to be determined by hidden variables.

**hidden-variable theories** Theories that use *hidden variables* in an attempt to avoid the *indeterministic* nature of *quantum mechanics*.

**Hilbert space** A special type of *inner product space* used implicitly in *quantum mechanics*, but not explicitly discussed in this course. Hilbert spaces include any finite-dimensional *vector space* (e.g. *spin space*) and certain infinite-dimensional vector spaces (e.g. *function space*). Strictly speaking, a Hilbert space must satisfy additional mathematical requirements, beyond those of a vector space. Intuitively, it should contain no holes; more precisely, given any infinite sequence of *vectors* whose differences become vanishingly small in *norm* as we progress along the sequence, we require that the limit of the sequence should be a vector in the Hilbert space. (This property is not explicitly used in this course.)

**hole** (B3: 189) In a *semiconductor*, *quantum states* in which *electrons* are missing from the *valence band* behave as if they contained positively-charged *particles* called holes.

**homonuclear diatomic molecule** (B3: 158) A *diatomic molecule* composed of two identical *nuclei*. *Molecular orbitals* of homonuclear diatomic molecules have either *even parity* or *odd parity* under the operation of *inversion* about the *centre of symmetry*, and are called respectively *gerade orbitals* or *ungerade orbitals*, labelled g and u.

**Hooke's law** (B1: 125) The force on a *particle* is said to obey Hooke's law if it is a *restoring force* (always acting towards the equilibrium position) and is proportional to the displacement of the particle from equilibrium. In one dimension, we write

$$F_x = -Cx,$$

where  $x$  is the displacement from the equilibrium position, and the proportionality constant  $C$  is called



the *force constant*. In *classical physics*, such a force leads to *simple harmonic motion*.

**horizontal polarization** Given a fixed axis perpendicular to the direction of propagation of *linearly-polarized light*, the *light* is said to be horizontally polarized relative to the given axis if its *electric field* is always perpendicular to that axis. Contrast with *vertical polarization*.

**Hund's rules** (B3: 138) Rules that allow us to determine the *energy ordering* of *atomic terms* and *atomic levels* arising from the same *electronic configuration*.

For atomic terms arising from the same electronic configuration, terms with higher values of the *total spin quantum number*  $S$  have lower energies. For atomic terms from the same configuration with the same value of  $S$ , those with higher values of the *total orbital angular momentum quantum number*  $L$  have lower energies.

For atomic levels arising from the same atomic term, the lowest level corresponds to the lowest *total angular momentum quantum number*  $J$  in a shell that is less than half full, and to the highest  $J$  in a shell that is more than half full. There is no *spin-orbit splitting* for a half-full shell.

Strictly speaking, Hund's rules apply only to *ground-state* configurations. They also apply to some *excited states*, but there are exceptional cases in which they fail.

**H/V basis** (B2: 178) A *basis* representing the *polarization states* of *photons* in which the *basis vectors* correspond to photons *linearly polarized* in vertical and horizontal directions. This is a *complementary basis* to the *diagonal basis*.

**hydrogen atom** An *atom* with *atomic number*  $Z = 1$  and therefore with one *proton* in its *nucleus* and a single *electron* outside the nucleus. Different *isotopes* of hydrogen have no *neutrons*, one neutron (*deuterium*) or two neutrons (*tritium*). Hydrogen *molecules* consist of two hydrogen atoms bound together.

**hydrogen molecule ion** (B3: 146) A *bound system* consisting of two *protons* and one *electron*.

**hydrogen-like atom** (B3: 91) A *bound system* composed of a negatively-charged *particle* and a positively-charged *nucleus*, interacting through the attractive *Coulomb force*.

**hydrogen-like system** A *bound system* composed of a negatively-charged *particle* and a positively-charged particle, interacting through the attractive *Coulomb force*.

**hyperbolic functions** (B1: 220) Functions that involve certain combinations of  $e^x$  and  $e^{-x}$ . For each trigonometric function involving a given combination

of  $e^{ix}$  and  $e^{-ix}$ , there corresponds a hyperbolic function with the same combination of  $e^x$  and  $e^{-x}$ . The hyperbolic cosine and hyperbolic sine functions are:

$$\cosh x = \frac{e^x + e^{-x}}{2}$$

$$\sinh x = \frac{e^x - e^{-x}}{2}.$$

**hyperfine structure** (B3: 107) Structure in the *energy levels* and the corresponding *spectral lines* of a *system* that is on an even smaller scale than *fine structure*.

In a *hydrogen atom*, hyperfine structure arises from the finite size of the *proton*, *quantum field theory* corrections such as the *Lamb shift* and interactions between the *magnetic dipole moments* of the *electron* and proton (not to be confused with the *spin-orbit interaction*).

**identical particles** (B2: 107) Two *particles* are identical if all their unchangeable attributes (such as *charge* and *mass*) are the same. For example, all *electrons* are identical, even if they are in different *spin states*.

**identity operator** (B1: 40; B2: 30) An *operator*  $\hat{I}$  that does not change the object on which it acts. Thus  $\hat{I}f(x) = f(x)$ .

**imaginary axis** (B1: 212) An axis in the *complex plane* along which *complex numbers* have zero *real part* and which points in the direction of increasing *imaginary part*.

**imaginary number** (B1: 210) A *complex number* of the form  $iy$ , where  $y$  is *real*. Compare with *imaginary part*.

**imaginary part** (B1: 210) Given a *complex number*  $z = x + iy$ , where  $x$  and  $y$  are *real numbers*, the imaginary part of  $z$  is equal to  $y$ . The imaginary part of any complex expression  $z$  is given by

$$\text{Im}(z) = \frac{z - z^*}{2i},$$

where  $z^*$  is the *complex conjugate* of  $z$ . Note that the imaginary part is a real number and does not include a factor of  $i$ .

**in phase** Two *oscillations* or *waves* are said to be in phase with one another if they permanently have the same *phase*.

**incompatible observables** (B2: 57) Two or more *observables* are said to be incompatible if they cannot all have definite values in the same *quantum state* (for a range of different values). The quantum-mechanical *operators* corresponding to a set of incompatible observables do not all *commute* with one another. Contrast with *compatible observables*.

**independent variable** In a function  $f(x, y, \dots, z)$ , the independent variables are  $x, y, \dots, z$ . Contrast with the *dependent variable*  $f$ .

**independent-particle model** (B3: 116) An approximation used to model *quantum states of electrons* in *atoms* in which electron–electron repulsion is neglected. The *time-independent Schrödinger equation* is then *separable*, allowing solutions to be found that are products of single-particle functions (*atomic orbitals*). Compare with *central-field approximation*.

**indeterministic** (B1: 13) A term indicating that identical *initial conditions* determine only the *probabilities* of various possible outcomes rather than guaranteeing the same outcome on all occasions. Indeterminism is a key feature of *quantum mechanics*. Contrast with *deterministic*.

**indistinguishable particles** *Particles* that are identical and cannot be distinguished from one another. *Identical particles* whose *wave functions* have overlapped, become *entangled*, and have not subsequently undergone a *state vector collapse*, are *indistinguishable*. Given a *system* of two such particles, we may be able to say that there is a particle in a given volume element, but we cannot say which of the particles this is.

**inelastic scattering** (B1: 196) *Scattering* for which *kinetic energy* is not conserved. In inelastic scattering, *particles* may change their *quantum state* of internal excitation or be absorbed; they may even be created or destroyed, especially at very high *energies*. Contrast with *elastic scattering*.

**inertial frame of reference** (B1: 127) A *frame of reference* set up and moving in such a way that all *free particles* have zero acceleration, in accordance with Newton’s first law. The laws of physics (including those of *classical mechanics* and *quantum mechanics*) are normally expressed in terms of observations made in inertial frames of reference.

**infinite square well** A *potential energy function* that is infinite everywhere except for a finite region, within which the potential energy has a constant value (which is usually taken to be zero).

In two and three dimensions, the region where the potential energy function is finite and constant may be of any shape; the ‘squareness’ refers to the abrupt discontinuity in the potential energy function not to the shape of the region in space. See *one-dimensional infinite square well*, *two-dimensional infinite square well* and *three-dimensional infinite square well*.

**infinite well** A *potential energy function* that has a minimum and increases to infinity in all directions away from the minimum. Examples include *infinite square wells* and the potential energy function of a *harmonic oscillator*. All the *energy eigenvalues*

in an infinite well are discrete and all the *energy eigenfunctions* describe *bound states*.

**initial conditions** (B1: 221) Conditions that supply extra information about the solution of a *differential equation* at a single value of the *independent variable*.

**inner product** (B2: 14, 75, 214) In a *vector space*, an inner product is a rule that combines two *vectors*  $|a\rangle$  and  $|b\rangle$  to produce a *scalar*  $\langle a|b\rangle$ , subject to the properties:

$$\langle b|a\rangle = \langle a|b\rangle^*,$$

$$\langle a|(|b\rangle + |c\rangle) = \langle a|b\rangle + \langle a|c\rangle,$$

$$\langle a|(\lambda|b\rangle) = \lambda\langle a|b\rangle, \quad \text{where } \lambda \text{ is a scalar,}$$

$$\langle a|a\rangle \geq 0, \quad \text{with equality only if } |a\rangle = |0\rangle.$$

The *Cauchy–Schwarz inequality* is a consequence of these defining properties.

For two vectors  $|f\rangle$  and  $|g\rangle$  in *function space*, the inner product is defined by the *overlap integral*

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x) g(x) dx.$$

For two vectors  $|A\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$  and  $|B\rangle = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$  in

*spin space*, the inner product is defined by

$$\langle A|B\rangle = \begin{bmatrix} a_1^* & a_2^* \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = a_1^* b_1 + a_2^* b_2.$$

In ordinary three-dimensional space, the inner product of two vectors is their *scalar product*.

**inner product space** (B2: 214) A *vector space* equipped with a specific *inner product*. *Function space* and *spin space* are both examples of inner product spaces.

**insulator** (B3: 186) In the context of electrical conduction, an insulator is a material that has a very low *electrical conductivity*. Insulators have large *band gaps* between the *valence band* and the *conduction band*, and have negligible concentrations of *donor atoms* or *acceptor atoms*. The band gap of a pure insulator is greater than about  $80kT$  at *absolute temperature*  $T$ , where  $k$  is *Boltzmann’s constant*; this corresponds to a band gap that is greater than about 2 eV at room temperature. Contrast with *conductor* and *semiconductor*.

**intensity of a beam** Another term for *beam intensity*. Compare with the *intensity of a wave*.

**intensity of a wave** For a classical *wave*, intensity is the amount of *energy* transported by the wave per unit time per unit area perpendicular to the direction of wave propagation. Intensity is proportional to the square of the *amplitude* of the wave. If a point source of waves radiates energy equally in all directions, the

intensity of the waves is inversely proportional to the square of the distance from the source. The *SI* unit of intensity is *watt* per square metre ( $\text{W m}^{-2}$ ).

**interatomic overlap integral** (B3: 149) The *overlap integral* of two *atomic orbitals* each based on a different *nucleus*.

**interference** (B1: 16) A phenomenon arising from the superposition of two or more *coherent waves*, resulting in a pattern of *interference maxima* and *interference minima*. See also *constructive interference* and *destructive interference*.

**interference maxima** (B1: 18) Features of *interference patterns* produced when two or more *coherent waves* interfere with one another. Interference maxima occur at points where the contributing waves reinforce one another, leading to a local maximum in the *intensity* of the wave (*constructive interference*).

**interference minima** (B1: 18) Features of *interference patterns* produced when two or more *coherent waves* interfere with one another. Interference minima occur at points where the contributing waves cancel one another, leading to a local minimum in the *intensity* of the wave (*destructive interference*).

**interference pattern** A pattern of peaks and troughs in *intensity* that occurs when *coherent waves* from a spatially extended source (or more than one source) are allowed to interfere with one another. See *interference*.

**interference rule** (B1: 32) A rule stating that, if a given process, leading from an initial *quantum state* to a final quantum state, can proceed in two or more alternative ways, and the way taken is not recorded, the *probability amplitude* for the process is the sum of the probability amplitudes for the different ways. When calculating the *probability* of the process, it is essential to add all the contributing probability amplitudes before taking the square of the *modulus*.

**intrinsic angular momentum** (B2: 73) Another term for *spin angular momentum*.

**inverse Fourier transform** (B1: 171) An operation that is the inverse of the *Fourier transform*. The inverse Fourier transform  $f(x)$  of a function  $A(k)$  is defined as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk.$$

The initial *wave function*  $\Psi(x, 0)$  of a *free particle* is the inverse Fourier transform of the *momentum amplitude*  $A(k)$ .

**inverse matrix** (B2: 223) The inverse of an  $n \times n$  *square matrix*  $A$  is another  $n \times n$  square matrix  $A^{-1}$  such that

$$AA^{-1} = A^{-1}A = I,$$

where  $I$  is an  $n \times n$  *unit matrix*.

**inversion** (B3: 22) The operation  $\mathbf{r} \rightarrow -\mathbf{r}$  is said to be an inversion about the origin. In *Cartesian coordinates*, this is the transformation  $x \rightarrow -x$ ,  $y \rightarrow -y$ ,  $z \rightarrow -z$ . In *spherical coordinates*, it is the transformation  $r \rightarrow r$ ,  $\theta \rightarrow \pi - \theta$ ,  $\phi \rightarrow \pi + \phi$ . Also called a *parity transformation*.

**ion** (B1: 12) An electrically-charged *atom* formed when a neutral atom loses or gains one or more *electrons* so that the *magnitude* of its total electronic charge is not equal to the magnitude of the charge of the *nucleus*.

**ionic bonding** (B3: 171) Bonding of *atoms* in a *molecule* or solid in which one type of atom loses one or more *electrons* and another type of atom gains them. The structure is held together by *electrostatic forces* between the resulting *ions*. Contrast with *covalent bonding* and *metallic bonding*.

**ionic crystal** (B1: 83) A crystal composed mainly of positive and negative *ions* held together by attractive *electrostatic forces* between ions of opposite sign. A familiar example is the crystal of common salt, NaCl.

**ionization** (B1: 11) The process in which a neutral *atom* loses one or more *electrons* to produce a positive *ion* and one or more unbound electrons.

**ionized** (B1: 11) The condition of an *atom* that has lost one or more *electrons*.

**isolated system** A *system* that is free from external influences. Such a system is not acted upon by external forces and exchanges no *energy* or matter with the rest of the Universe.

**isotope** (B1: 13) Isotopes of a given *element* are *atoms* or *nuclei* with the same number of *protons*, and therefore the same *atomic number*,  $Z$ . Different isotopes have different numbers of *neutrons*, and therefore different *mass numbers*,  $A$ .

The usual symbol for an isotope is  ${}^A\text{Sy}$ , where Sy is the chemical symbol for the element. Since Sy determines  $Z$ , the fuller notation  ${}_Z^A\text{Sy}$  is strictly redundant, but may be helpful for elements for which  $Z$  is not widely-remembered. For example, the isotope of silicon with  $A = 27$  and  $Z = 14$  can be written as  ${}^{27}\text{Si}$  or  ${}_{14}^{27}\text{Si}$ . Less formally, this isotope is referred to as silicon-27.

**jj-coupling scheme** (B3: 138) A scheme for determining the *total angular momentum* of an *atom*. The *orbital angular momentum* and *spin angular momentum* of each *electron* are combined to find the electron's total angular momentum. The total angular momentum of the atom is then found by adding together contributions from each electron. This scheme applies to atoms with large *atomic number* ( $Z \geq 80$ ). Contrast with the *LS-coupling scheme*.



**kelvin** The unit of temperature on the *absolute temperature scale*, represented by the symbol K. This is the *SI* unit of temperature. A temperature difference of one kelvin (1 K) is equivalent to a temperature difference of one degree Celsius (1 °C), but the two scales have different zeros, with zero kelvin corresponding to *absolute zero*, the lowest conceivable temperature for a *system* in equilibrium.

**ket vector** (B2: 13, 20) A *vector*  $|g\rangle$  which forms the right-hand part of a *Dirac bracket*  $\langle f|g\rangle$ . The ket vector  $|g\rangle = \sum_i c_i |g_i\rangle$ , where the  $c_i$  are *complex numbers*, can be joined to any *bra vector*  $\langle f|$  to give

$$\langle f|g\rangle = \sum_i c_i \langle f|g_i\rangle.$$

**key distribution problem** (B2: 181) The problem of sending a *cryptographic key* without the possibility of undetected eavesdropping.

**kinetic energy** *Energy* due to motion. The kinetic energy of a *particle* is given by

$$E_{\text{kin}} = \frac{1}{2}mv^2 = \frac{p^2}{2m},$$

where  $m$  is the mass of the particle,  $v$  is its speed and  $p$  is the *magnitude* of its *momentum*.

**kinetic energy operator** (B1: 44) The quantum-mechanical *operator* representing the *kinetic energy* of a *system*. In one dimension, a *particle* of mass  $m \neq 0$  has the kinetic energy operator

$$\hat{E}_{\text{kin}} = \frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}.$$

**Kronecker delta symbol** (B1: 103) The symbol  $\delta_{ij}$  that represents 1 if  $i = j$ , and represents 0 if  $i \neq j$ . Thus,

$$\sum_i a_i \delta_{ij} = a_j.$$

**ladder operator** (B1: 140) A term used to describe the *raising operator* or the *lowering operator* of a *harmonic oscillator*.

**Lamb shift** (B3: 111) A very small *energy* splitting between the  $n = 2, l = 0, j = \frac{1}{2}$  *quantum state* and the slightly higher  $n = 2, l = 1, j = \frac{1}{2}$  *quantum state* in a *hydrogen atom*. This forms part of the *hyperfine structure* of the hydrogen atom and is accurately explained by *quantum electrodynamics*.

**Laplacian operator** (B3: 13) The partial differential *operator*, given in *Cartesian coordinates* by

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2},$$

and in *spherical coordinates* by

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \phi}.$$

**Larmor frequency** (B2: 91) For a *spin- $\frac{1}{2}$  particle* with *spin gyromagnetic ratio*  $\gamma_s$  in a *magnetic field* of *magnitude*  $B$ , the Larmor frequency is

$$\omega = |\gamma_s|B.$$

*Spin states* that are *spin-up* and *spin-down* relative to the magnetic field have their *energies* separated by  $\hbar\omega$ , where  $\hbar$  is *Planck's constant* divided by  $2\pi$ . *Spin components* perpendicular to the magnetic field have *expectation values* that vary sinusoidally at an *angular frequency* equal to the Larmor frequency.

**laser** A device which when stimulated with incident *electromagnetic radiation* produces an intense source of *coherent light* in the form of a narrow beam. The word ‘laser’ is an acronym for Light Amplification by the *Stimulated Emission* of Radiation.

**lattice** (B3: 170) A periodically-repeated three-dimensional array of *lattice points*, used to specify the positions of *atoms* or *ions*, or groups of atoms or ions, in a *crystal*.

**lattice point** (B3: 170) One of the points in a *lattice*. All lattice points in a given lattice have exactly the same environment.

**lattice translation operator** (B3: 177) For a given *lattice vector*  $\mathbf{R}$ , an *operator*  $\hat{T}(\mathbf{R})$  which has the effect

$$\hat{T}(\mathbf{R})\psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R})$$

when applied to any function  $\psi(\mathbf{r})$ .

The fact that all lattice translation operators *commute* with one another and with the *Hamiltonian operator* of an infinite crystal leads to *Bloch's theorem*.

**lattice vector** (B3: 170) A *displacement vector* that joins two points in a *lattice*.

**LCAO approximation** (B3: 148) An abbreviation for the method of *linear combination of atomic orbitals*.

**left-handed circular polarization** See *circular polarization*.

**length parameter** (B1: 133) For a *harmonic oscillator*, the length parameter is

$$a = \sqrt{\frac{\hbar}{m\omega_0}},$$

where  $\hbar$  is *Planck's constant* divided by  $2\pi$ ,  $m$  is the mass of the oscillating *particle*,  $\omega_0 = \sqrt{C/m}$  is the classical *angular frequency* and  $C$  is the *force constant* of the oscillator.

The length parameter characterizes the quantum properties of the oscillator. For example, in a *state* with *quantum number*  $n$ , the *uncertainties* in position

and *momentum* are given by  $(n + \frac{1}{2})^{1/2}a$  and  $(n + \frac{1}{2})^{1/2}\hbar/a$ , respectively.

**levels** See *atomic levels*.

**light** A term normally reserved for *visible light*, but sometimes used for any type of *electromagnetic radiation*.

**linear combination** Given a set of functions  $f_1(x)$ ,  $f_2(x)$ , ..., and a set of (possibly *complex*) constants  $c_1, c_2, \dots$ , any expression of the form

$$c_1 f_1(x) + c_2 f_2(x) + \dots$$

is called a linear combination of  $f_1(x)$ ,  $f_2(x)$ , ...

BOOK 2: This concept can be generalized to other sums. For example, an expression of the form

$$c_1|a_1\rangle + c_2|a_2\rangle + \dots$$

is a linear combination of *vectors*. Also called *linear superposition*.

**linear combination of atomic orbitals** (B3: 148)

An approximation method used to find approximate *molecular orbitals* and *electronic energies* in molecules and solids within the *Born–Oppenheimer approximation*. For a *diatomic molecule*, a *trial function* is constructed as a *linear combination* of *atomic orbitals*, centred on the two *nuclei*, with the same values of  $|m|$ , where  $m$  is the *azimuthal quantum number*. The *variational method* is then used to estimate the electronic energies and to find the corresponding molecular orbitals.

In the *tight-binding method* for the *states* of *electrons* in *crystalline solids*, a linear combination of atomic orbitals is used that satisfies *Bloch's theorem*.

**linear differential equation** (B1: 217) An *ordinary differential equation* of the form

$$\hat{L}y(x) = f(x),$$

where  $\hat{L}$  is a *linear differential operator*.

**linear differential operator** (B1: 218) A *linear operator* of the form

$$\hat{L} = a_n(x) \frac{d^n}{dx^n} + a_{n-1}(x) \frac{d^{n-1}}{dx^{n-1}} + \dots + a_1(x) \frac{d}{dx} + a_0(x),$$

where  $a_n(x), a_{n-1}(x) \dots a_0(x)$  are functions of  $x$  (some of which may be constant or equal to zero). A *linear differential equation* can be written in the form  $\hat{L}y(x) = f(x)$ , where the special case  $\hat{L}y(x) = \lambda y(x)$  is an *eigenvalue equation*.

**linear Hermitian operator** A *linear operator* that is also a *Hermitian operator*.

**linear homogeneous differential equation** (B1: 218)

An ordinary or partial *linear differential equation* in which each term is proportional to the *dependent variable* or one of its derivatives with respect to the *independent variable*, and there is no term that is a

constant or that depends only on the independent variable. For example,

$$\frac{d^2 y(x)}{dx^2} + \sin(2x) y(x) = 0$$

is a linear homogeneous differential equation with dependent variable  $y$  and independent variable  $x$ .

*Eigenvalue equations* of the form  $\hat{L}f(x) = \lambda f(x)$ , where  $\hat{L}$  is a *linear differential operator* are examples of linear homogeneous differential equations. The solutions of linear homogeneous differential equations obey the *principle of superposition*.

**linear number density** (B1: 183) The number of specified entities (e.g. *atoms*) per unit length, along a given line. The *SI* unit of linear number density is  $m^{-1}$ . Do not confuse linear number density with *number density*, which is a different quantity with different units.

**linear operator** (B1: 42) An *operator*  $\hat{O}$  that satisfies the condition

$$\hat{O}[\alpha f(x) + \beta g(x)] = \alpha \hat{O}f(x) + \beta \hat{O}g(x)$$

for arbitrary *complex* constants  $\alpha$  and  $\beta$ .

In *quantum mechanics*, all *observable* quantities are represented by linear operators.

BOOK 2: See also *Hermitian operators*.

**linear polarization** (B2: 163) In *classical physics*, *electromagnetic radiation* is said to have linear polarization if its *electric field vector* oscillates in a fixed plane that contains the direction of propagation of the radiation. In *quantum physics*, the corresponding *photons* are also said to be *linearly polarized*. Contrast with *circular polarization*.

**linear polarization matrix** (B2: 176) A *matrix*

$$\hat{\mathcal{P}}(\theta) = \begin{bmatrix} \cos(2\theta) & \sin(2\theta) \\ \sin(2\theta) & -\cos(2\theta) \end{bmatrix},$$

whose *eigenvectors*  $|V_\theta\rangle$  and  $|H_\theta\rangle$  represent *polarization states* of *photons* that are *linearly polarized* at an angle  $\theta$  to the vertical and horizontal directions, which we take to be the positive  $z$ - and  $x$ -directions. The angle  $\theta$  is then the *polar angle* in *spherical coordinates* with *azimuthal angle*  $\phi = 0$ ; so  $\theta$  is measured from the positive  $z$ -axis towards the positive  $x$ -axis.

The eigenvectors of  $\hat{\mathcal{P}}(\theta)$  are

$$|V_\theta\rangle = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix} \quad \text{and} \quad |H_\theta\rangle = \begin{bmatrix} -\sin \theta \\ \cos \theta \end{bmatrix},$$

with *eigenvalues*  $+1$  and  $-1$ , respectively.

**linear superposition** An alternative term for *linear combination*.

**linearly polarized** (B2: 163) The condition of having *linear polarization*.

**local hidden variables** *Hidden variables* that are consistent with the principle of *locality*. At time  $t$ , the

value of a local hidden variable describing a given *particle* cannot be influenced by an event that occurs at a distance  $L$  from the particle at any time later than  $t - L/c$ , where  $c$  is the *speed of light* in a vacuum.

**local hidden-variable theories** (B2: 161) Theories based on *local hidden variables* in accordance with the principles of *realism* and *locality*. In a local hidden-variable theory, each of two well-separated *particles* is supposed to have its own hidden variables which, if known, determine all the *observable* properties of the particle. *Bell's theorem* shows that such theories cannot reproduce all the results of *quantum mechanics*. Experimental evidence appears to confirm the predictions of quantum mechanics and refute the predictions of local hidden-variable theories.

**local-realism** (B2: 161) A term given to the combined assumptions of *locality* and *realism* that characterize *local hidden-variable theories*.

**locality** (B2: 161) The assertion that event A, occurring at time  $t_A$ , cannot influence event B, occurring at time  $t_B$ , if  $t_A > t_B - L/c$ , where  $L$  is the distance between the two events and  $c$  is the *speed of light* in a vacuum. This principle is consistent with special relativity.

**longitudinal wave** A wave composed of *oscillations* that take place in a direction parallel to the direction of propagation of the wave. Contrast with *transverse wave*.

**lowering operator** (B1: 137) For a *harmonic oscillator* with *length parameter*  $a$ , the lowering operator is defined as

$$\hat{A} = \frac{1}{\sqrt{2}} \left( \frac{x}{a} + a \frac{\partial}{\partial x} \right),$$

For  $n \geq 1$ , this *operator* converts an *energy eigenfunction*  $\psi_n(x)$  of the oscillator into the next eigenfunction of lower *energy*, while  $\hat{A}\psi_0(x) = 0$ . If the eigenfunctions are *normalized*,

$$\hat{A}\psi_n(x) = \sqrt{n}\psi_{n-1}(x) \quad \text{for } n = 1, 2, \dots$$

See also *raising operator* and *ladder operator*.

**LS-coupling scheme** (B3: 137) A scheme for determining the *total angular momentum* of an *atom*. The *orbital angular momenta* of all the *electrons* are combined to give the *total orbital angular momentum*,  $\mathbf{L}$ . The *spin angular momenta* of all the electrons are combined to give the *total spin angular momentum*,  $\mathbf{S}$ . The total angular momentum of the atom,  $\mathbf{J}$ , is then found by adding the total orbital angular momentum and total spin angular momentum:  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ . This scheme applies to atoms of small *atomic number* ( $Z \leq 35$ ). Contrast with the *jj-coupling scheme*.

**Mach-Zehnder interferometer** (B1: 32) An arrangement of two *half-silvered mirrors*, which act as

*beam splitters*, two fully-reflecting mirrors, and two detectors, which is used to demonstrate *interference* phenomena in *light*. These interference phenomena are evident even if only one *photon* passes through the Mach-Zehnder interferometer at a time.

**macroscopic wave function** (B2: 121) A *wave function*  $\Psi(\mathbf{r}, t)$  that depends on a single position *vector* and describes the behaviour of a *Bose-Einstein condensate*. The *number density* of *particles* in the condensate is given by  $|\Psi(\mathbf{r}, t)|^2$ .

**magnetic dipole** (B2: 43) An entity that has magnetic properties like those of a tiny magnet or loop of *electric current* and is characterized by a *magnetic dipole moment*.

**magnetic dipole moment** (B2: 43) A *vector* quantity  $\boldsymbol{\mu}$  that characterizes the magnetic properties of a *magnetic dipole*. The potential energy of a magnetic dipole in a *magnetic field*  $\mathbf{B}$  is  $E_{\text{mag}} = -\boldsymbol{\mu} \cdot \mathbf{B}$ . The torque on the magnetic dipole is  $\boldsymbol{\Gamma} = \boldsymbol{\mu} \times \mathbf{B}$ . In a non-uniform magnetic field  $\mathbf{B}$ , a magnetic dipole experiences a force  $\mathbf{F} = \nabla(\boldsymbol{\mu} \cdot \mathbf{B})$ .

**magnetic field** A *vector* field which determines the *magnetic force* on a charged *particle* moving through a given point. The magnetic field at a point P is a vector quantity  $\mathbf{B}$  such that the magnetic force on a particle of *charge*  $q$ , passing through P with velocity  $\mathbf{v}$ , is given by the *vector product*

$$\mathbf{F} = q(\mathbf{v} \times \mathbf{B}).$$

**magnetic force** A velocity-dependent force experienced by a *particle* with an *electric charge* moving in a *magnetic field*. The force is perpendicular to both the velocity of the particle and the magnetic field, and is given by the *vector product*

$$\mathbf{F} = q(\mathbf{v} \times \mathbf{B}),$$

where  $q$  is the particle's *charge*,  $\mathbf{v}$  is its velocity and  $\mathbf{B}$  is the magnetic field at the position of the particle.

**magnetic quantum number** (B2: 51; B3: 10) The *quantum number*  $m$  that determines the value of the  $z$ -component of *orbital angular momentum*:  $L_z = m\hbar$ , where  $\hbar$  is *Planck's constant* divided by  $2\pi$ . In all cases,  $m$  is an integer:  $m = 0, \pm 1, \pm 2, \dots$ . For a fixed value of the *orbital angular momentum quantum number*,  $l$ , the magnetic quantum number is restricted to the values  $m = -l, -l + 1, \dots, l - 1, l$ . Also called the *azimuthal quantum number*.

**magnitude** (B2: 16, 205) A non-negative *real* quantity. The magnitude of a *scalar*  $Q$  is a non-negative quantity  $|Q|$  describing the size of  $Q$ , irrespective of its sign. The magnitude of a *vector*  $\mathbf{a}$  is a non-negative quantity  $|\mathbf{a}|$ , describing the size of  $\mathbf{a}$ , irrespective of its direction; this is usually written as  $a$ , omitting both the bold print and the modulus signs.

BOOK 2: The magnitude of an *abstract vector* is generally called its *norm*.



**Malus's law** (B2: 164) Classically, Malus's law states that the *intensity* of *light* passing sequentially through two *polarization preparers* oriented at a relative angle of  $\theta$  varies as  $\cos^2 \theta$ . Quantum mechanically, a *photon* that is transmitted through one polarization preparer, has a *probability*  $\cos^2 \theta$  of passing through a second polarization preparer oriented at an angle  $\theta$  relative to the first. Compare with the  $\cos^2(\theta/2)$  rule.

**mass number** (B3: 95) The total number of *neutrons* and *protons* in a *nucleus*,  $A = N + Z$ , where  $N$  is the number of neutrons and  $Z$  is the number of protons (the *atomic number*).

**matrix** (B2: 215) A set of objects (called *matrix elements*) arranged in a rectangular pattern of rows and columns, with special rules for addition, multiplication by a *scalar* and the multiplication of matrices.

**matrix eigenvalue equation** (B2: 224) An *eigenvalue equation* of the form

$$AX = \lambda X,$$

where  $A$  is a  $n \times n$  *square matrix*,  $X$  is a  $n \times 1$  non-zero *column matrix*, and  $\lambda$  is an undetermined *scalar*.

**matrix element** (B2: 215, 220; B3: 204) (i) In mathematics, the  $ij$ -matrix element of a *matrix*  $A$  is the *scalar*  $A_{ij}$  that appears in the  $i$ th row and  $j$ th column of the matrix.

(ii) In *quantum mechanics*, given an *operator*  $\hat{A}$  and a set of *basis vectors*  $|e_n\rangle$ , the  $ij$ -matrix element of  $\hat{A}$  is given by  $\langle e_i | \hat{A} | e_j \rangle$ . For example, given a basis of *energy eigenfunctions*  $\psi_n(x)$ , the  $ij$ -matrix element of the operator  $\hat{A}$  is

$$A_{ij} = \int_{-\infty}^{\infty} \psi_i^*(x) \hat{A} \psi_j(x) dx.$$

**maximally-entangled states** (B2: 185) For *photons* or *spin- $\frac{1}{2}$  particles*, another term for *Bell states*.

**Maxwell's equations** (B1: 17) A set of four *partial differential equations* relating the *electric field*  $\mathbf{E}(\mathbf{r}, t)$  and *magnetic field*  $\mathbf{B}(\mathbf{r}, t)$  to each other and to their sources in *electric charges* and *currents*. These are the basic field equations of classical electromagnetism.

**mean value** (B1: 111, 228) An alternative term for *average value*.

**measurement** In *quantum mechanics*, a measurement is an interaction or communication of information between a *quantum system* and a classical measuring device. The measurement occurs when a quantum system causes some sort of irreversible change in the measuring device, and possibly in its surroundings, and the system undergoes a *collapse of the wave function*. BOOK 2: More generally, the system undergoes a *state vector collapse*.

**metallic bonding** (B3: 171) The type of bonding found in metals. Many *atoms* contribute to the bonding, not just nearest neighbours, and the *valence electrons* have a *probability density* that spreads out over the whole material. The atomic cores are bathed in a sea of *electrons* that are free to flow throughout the metal. Contrast with *ionic bonding* and *covalent bonding*.

**modulus** (B1: 210) For any *complex number*  $z = x + iy$ , the modulus is the non-negative *real number*

$$|z| = \sqrt{x^2 + y^2},$$

where  $x$  is the *real part* and  $y$  is the *imaginary part* of  $z$ . If the complex number is written in *polar form*  $z = r(\cos \theta + i \sin \theta)$  or in *exponential form*  $z = re^{i\theta}$ , the modulus is equal to  $r$ . For any complex expression,  $|z| = \sqrt{zz^*}$ .

**molecular orbital** (B3: 148, 157) The *eigenfunction* of a single-particle *time-independent Schrödinger equation* used to model the *state* of an *electron* in a *molecule*. The *LCAO approximation* provides a good approximation for molecular orbitals.

**molecule** Traditionally, the smallest part of a pure substance that retains the chemical identity of that substance. From a microscopic point of view, a molecule is a particular group of *atoms* bound together in a particular way.

**moment of inertia** (B2: 42) A quantity that represents the reluctance of a body to depart from a state of constant *angular momentum* along a given axis. For a fixed axis of rotation, the moment of inertia is defined by

$$I = \sum_i m_i d_i^2,$$

where the  $m_i$  is the mass of *particle*  $i$ ,  $d_i$  is the distance of particle  $i$  from the axis of rotation, and the sum is over all the particles in the body.

The rotational *energy levels* of a *diatomic molecule* are given by

$$E_{\text{rot}} = \frac{1}{2I} l(l+1) \hbar^2,$$

where  $l$  is the *orbital angular momentum quantum number*,  $\hbar$  is *Planck's constant* divided by  $2\pi$  and  $I$  is the moment of inertia of the molecule about an axis along the line joining its *atoms*.

**momentum** A *vector* quantity describing of the amount of translational motion of a *particle* or *system*. In *classical mechanics*, the momentum of a particle is

$$\mathbf{p} = m\mathbf{v},$$

where  $m$  is the particle's mass and  $\mathbf{v}$  is its velocity. The momentum of a system of particles is the vector sum of the momenta of all the particles. The *SI* unit of momentum is  $\text{kg m s}^{-1}$ .

**momentum amplitude** (B1: 170) A quantity whose *modulus squared* gives the *probability distribution* of *momentum* via *Born's rule for momentum*.

For a *free particle* in one dimension, the momentum amplitude  $A(k)$  is the function that appears in the expansion of a free-particle *wave function*  $\Psi(x, t)$  in terms of *de Broglie wave functions*:

$$\Psi(x, t) = \int_{-\infty}^{\infty} A(k) e^{i(kx - E_k t/\hbar)} dx.$$

It is given by the *Fourier transform* of the initial free-particle wave function:

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, 0) e^{-ikx} dx$$

For non-free particles, the momentum amplitude  $A(k, t)$  depends on time and is given by the Fourier transform of the wave function,  $\Psi(x, t)$ . Also called the *momentum wave function*.

**momentum eigenfunction** (B1: 168) For a single *particle* in one dimension, an *eigenfunction* of the *momentum operator* conventionally represented as

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx},$$

where  $k$  is a *real* constant called the *wave number* and the corresponding *eigenvalue* is  $\hbar k$ . The factor  $1/\sqrt{2\pi}$  is included by convention so that the *Fourier transform* of any function  $\phi(x)$  is simply expressed as  $\langle \psi_k | \phi \rangle$ .

**momentum operator** (B1: 44) The quantum-mechanical *operator* representing the *momentum* of a *system*. For a single *particle* in one dimension, the momentum operator is

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}.$$

**momentum wave function** (B1: 170) Another term for the *momentum amplitude*.

**multiplicity** (B3: 136) In the *LS-coupling scheme*, an *atomic term* with *total orbital angular momentum quantum number*  $L$  and *total spin quantum number*  $S$ , has multiplicity of  $2S + 1$ ; this is the number of different  $M_S$  values associated with the given value of  $S$ . For  $L \geq S$  (only) the multiplicity is the number of different  $J$  values associated with the atomic term, and is therefore the number of *atomic levels* into which the atomic term splits as a result of the *spin-orbit interaction*.

**muon** (B3: 93) An *elementary particle* with the same *charge* as an *electron* and a mass that is 207 times greater than the mass of an electron. The muon has a *half-life* of  $2.2 \times 10^{-6}$  s and decays into an electron plus a neutrino–antineutrino pair.

**muonic atom** (B3: 94) An *atom* in which a negatively-charged *muon* is bound to the *nucleus*.

Muonic atoms provide useful information about the distribution of *protons* in nuclei.

**mutually exclusive outcomes** (B1: 228) A set of outcomes such that the occurrence of one of them in a given measurement implies that none of the others occur in that measurement. The *probability* that one or other of a set of mutually exclusive outcomes will occur is found by adding their individual probabilities. This is the *addition rule for probability*.

**n-type semiconductor** (B3: 191) A *semiconductor* that has been *doped* with a sufficient number of *donor atoms* for its electrical behaviour to be dominated by negatively-charged *electrons* in the *conduction band*. Contrast with *p-type semiconductor*.

**neutron** An electrically-neutral *elementary particle* which is a constituent of all atomic *nuclei* (except the common form of *hydrogen*). A neutron has a mass slightly greater than that of a *proton*, it has no net *charge*, but it does have a *magnetic dipole moment*. The neutron is stable within an atomic nucleus, but is unstable in a vacuum where it has a *half-life* of 914 s.

**no-cloning theorem** (B2: 191) The quantum-mechanical theorem establishing that it is impossible to clone an arbitrary unknown *state* of a *quantum system*. This theorem prevents some proposed attacks on *protocols* for *quantum key distribution* and undermines simplistic proposals for *quantum teleportation* without *entanglement*.

**noble gases** (B3: 129) *Chemical elements* in the *group* on the extreme right of the *Periodic Table*, namely *helium* (He), *neon* (Ne), *argon* (Ar), *krypton* (Kr), *xenon* (Xe) and *radon* (Rn). In noble gas *atoms*, all the *shells* up to a given value of the *principal quantum number*  $n$  are *closed*. This makes noble gas atoms very non-reactive, with little tendency to form *molecules* with other atoms.

**nodal surface** (B3: 57) A surface on which a function vanishes. For example, the  $2s$  *energy eigenfunction* in a *hydrogen atom* has a spherical nodal surface.

**nodes** (B1: 73) Fixed points of zero disturbance in a *standing wave* (excluding points on the boundaries of the region where the disturbance takes place).

**non-commuting matrices** (B2: 217) Two *matrices*  $A$  and  $B$  are non-commuting if  $AB \neq BA$ .

**non-degenerate** A set of *stationary states* or *energy eigenfunctions* is said to be non-degenerate if all members of the set correspond to different *energies*. An *energy level* that corresponds to only one *quantum state* is also said to be non-degenerate. Contrast with *degenerate*.

**non-equivalent electrons** *Electrons* in an *atom* that belong to different *shells*, and so have different values of either the *principal quantum number*  $n$  or the

*orbital angular momentum quantum number*  $l$ .  
Contrast with *equivalent electrons*.

**non-local effects** (B2: 147) Non-local effects are said to occur when an event appears to be affected by events that happen at other points that are too far away for any communication to take place, even at the *speed of light*.

**norm** (B2: 16) The norm of an *abstract vector*  $|f\rangle$  in a *vector space* is given by  $\sqrt{\langle f|f\rangle}$ , the positive square root of the *inner product* of the vector with itself.

**normal ordering** (B1: 138) The conventional ordering  $\hat{A}^\dagger \hat{A}$  for the *raising* and *lowering operators* of a *harmonic oscillator*. These *operators* do not *commute* with one another so their order matters. In fact, we have  $\hat{A}\hat{A}^\dagger = \hat{A}^\dagger \hat{A} + \hat{I}$ , where  $\hat{I}$  is the *identity operator*.

**normalizable function** In one dimension, a function  $f(x)$  is said to be normalizable if

$$0 < \int_{-\infty}^{\infty} |f(x)|^2 dx < \infty.$$

A normalizable function can be converted into a *normalized function* by multiplying it by a suitable *normalization constant*.

**normalization condition** (B1: 50) A condition, based on *Born's rule*, which requires that the *probability* of finding a given *particle* to be somewhere in the whole of space is equal to 1. For a single particle in one dimension, in a *state* described by the *wave function*  $\Psi(x, t)$ , the normalization condition takes the form

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1.$$

By convention, *bound state energy eigenfunctions*  $\psi_n(x)$  also obey a normalization condition:

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = 1.$$

Similar normalization conditions apply to *systems* of more than one particle in more than one dimension.

BOOK 2: In *Dirac notation*, the normalization condition is written as  $\langle \Psi | \Psi \rangle = 1$ , and this applies to all *state vectors*, including those describing *spin states*.

**normalization constant** (B1: 50) A constant  $A$  chosen so that, if  $\Phi(x, t)$  is a *normalizable wave function*, then  $\Psi(x, t) = A\Phi(x, t)$  is a *normalized wave function*. Because any overall *phase factor* multiplying a wave function has no physical significance, the normalization constant of a one-dimensional *system* may be taken to be the *real positive constant*

$$A = \left( \int_{-\infty}^{\infty} |\Phi(x, t)|^2 dx \right)^{-1/2}.$$

This turns out to be independent of time. This result can be extended to *energy eigenfunctions* and to systems of more than one *particle* in more than one dimension.

**normalization integral** In one dimension, an integral of the form

$$\int_{-\infty}^{\infty} |f(x)|^2 dx$$

that must be set equal to 1 to ensure that the function  $f(x)$  is *normalized*.

**normalization rule** (B1: 228) A mathematical rule setting the scale for the *probabilities* of outcomes in a discrete *complete set* of *mutually exclusive outcomes*. The probabilities obey the rule

$$\sum_i p_i = 1,$$

where the sum is over all the outcomes in the set.

This condition can be extended to a *real variable*  $x$  with a *continuous probability distribution*. In this case,

$$\int_{-\infty}^{\infty} \rho(x) dx = 1,$$

where  $\rho(x)$  is the *probability density function* for the variable  $x$ .

**normalized** (B1: 50) A term used to describe a *wave function* or *eigenfunction* that satisfies the *normalization condition*. See also *normalized vector*.

**normalized vector** (B2: 16, 208) A *vector* of unit *norm*. A vector  $|a\rangle$  in a *vector space* is normalized if the *inner product*  $\langle a|a\rangle = 1$ .

**$n$ th-order approximation** (B3: 80) See *order of approximation*.

**nuclear fusion** A process in which two *nuclei* fuse together to form a larger nucleus. If the final nucleus has *mass number*  $A \leq 56$  or thereabouts (e.g.  $^{56}\text{Fe}$ ), the mass of the final nucleus is less than the sum of the masses of the initial nuclei, and *energy* is released. Fusion reactions often proceed by quantum-mechanical *tunnelling*.

In stars, fusion is crucial for energy release and for the conversion of primordial *hydrogen* into other light *elements*, from *helium* up to iron. Fusion reactions are also the basis for the energy released in hydrogen bombs.

**nuclear time-independent Schrödinger equation** (B3: 145) A *time-independent Schrödinger equation* that describes the behaviour of the *nuclei* in a *molecule* in the *Born–Oppenheimer approximation*. The *potential energy* term in the equation is called the *total static energy*; this is the sum of the *electronic energy* and the mutual potential energy of the nuclei.

**nuclei** The plural of *nucleus*.



**nucleus** The positively-charged, very compact central part of an *atom*, composed of *protons* and *neutrons*. The nucleus is some  $10^4$  times smaller in radius than an atom, but contains nearly all the mass. The number of positively-charged protons in the nucleus of a given *element* is equal to the *atomic number*,  $Z$ .

**number density** The number of specified entities (e.g. *atoms*) per unit volume.

**number operator** (B1: 141) The operator  $\hat{A}^\dagger \hat{A}$ , where  $\hat{A}^\dagger$  is the *raising operator* and  $\hat{A}$  is the *lowering operator* for a *harmonic oscillator*. When the number operator acts on an *energy eigenfunction* of the harmonic oscillator, it gives the *eigenvalue equation*

$$\hat{A}^\dagger \hat{A} \psi_n(x) = n \psi_n(x),$$

where  $n = 0, 1, 2, \dots$  is the *quantum number* of the eigenfunction  $\psi_n(x)$ .

**observable** (B1: 44; B2: 22) Any quantity that can be measured. In *quantum mechanics*, each observable quantity is represented by a *linear operator*.

BOOK 2: In more detail, observable quantities are represented by *linear Hermitian operators*; the Hermitian property ensures that these operators have *real eigenvalues* and *real expectation values*.

**odd function** (B1: 78) A function  $f(x)$  for which  $f(-x) = -f(x)$  for all  $x$ . Compare with *even function*.

**odd parity** (B3: 22) A function is said to have odd parity if it keeps the same *magnitude* but reverses sign under the operation of *inversion*. Equivalently, it is said to have *parity*  $-1$ . Compare with *odd function*. Contrast with *even parity*.

**old quantum theory** (B1: 7) A term given to attempts made between 1900 and 1925 to reconcile quantum concepts with *classical physics*. The resulting theory was based on ad-hoc ideas and never became a comprehensive world-view. While it had successes (the *Bohr model* explained the *spectral lines* of *hydrogen atoms*) it ran into serious difficulties (failing to explain the spectral lines of *helium atoms*, for example). Old quantum theory was superseded by *quantum mechanics* in the period from 1924 to 1927.

**one-dimensional infinite square well** (B1: 65) A one-dimensional *potential energy function* that is infinite everywhere except for a finite region, within which the *potential energy* has a constant value (usually taken to be zero). In a one-dimensional infinite square well of width  $L$ , with zero potential energy within the well, a *particle* of mass  $m$  has *energy eigenvalues*

$$E_n = \frac{n^2 \hbar^2}{2mL^2},$$

where the *quantum number*  $n$  is a positive integer. The *energy eigenfunctions* are *sinusoidal functions* and there is no *degeneracy* in this case.

**one-electron atom** An *atom* or *ion* with a single *electron*. Examples include *hydrogen*, singly-ionized *helium*, doubly-ionized *lithium*, and so on.

**one-time pad** (B2: 180) A randomly-chosen *cryptographic key* that is as long as the message that is to be encoded, and which is used to encode and decode only one message. Messages sent with one-time pads cannot be deciphered by anyone who does not have the key.

**open shell** (B3: 127) A *shell* in an *atom* that holds less than its capacity of  $2 \times (2l + 1)$  *electrons*. For example, a 2p-shell is open if it contains fewer than six electrons. Contrast with *closed shell*.

**operator** (B1: 40) In the context of functions, an operator is a mathematical entity that acts on a function to produce another function. It is conventional to indicate an operator by putting a hat on it, as in  $\hat{O}$ . Examples of such operators include the *momentum operator*  $\hat{p}_x = -i\hbar \partial/\partial x$ , the *position operator*  $\hat{x} = x$  and the *Hamiltonian operator*,  $\hat{H}$ , which represents the total *energy* of the *system*.

BOOK 2: In the context of *matrices*, an operator is a *square matrix* that acts on a *column matrix* to produce another column matrix. In a *vector space*, an operator is an entity that acts on a *vector* to produce another vector.

**orbital** (B3: 117, 148, 157) An *eigenfunction* of a single-particle *time-independent Schrödinger equation*, describing the *state* of an *electron* in an *atom* or *molecule*. See *atomic orbital* and *molecular orbital*.

**orbital angular momentum** (B2: 40) *Angular momentum* associated with the motion of a *particle*, or a *system* of particles, through space. This includes the angular momentum associated with a rigid body that is rotating about a fixed axis, and all the other usages of angular momentum in *classical physics*. It does not include the quantum-mechanical concept of *spin angular momentum*.

**orbital angular momentum operators** In *Cartesian coordinates*, the operators for the components of the *orbital angular momentum* of a *particle* are:

$$\begin{aligned}\hat{L}_z &= -i\hbar \left[ x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right], \\ \hat{L}_x &= -i\hbar \left[ y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right], \\ \hat{L}_y &= -i\hbar \left[ z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right].\end{aligned}$$

where  $\hbar$  is *Planck's constant* divided by  $2\pi$ . In

spherical coordinates,

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}.$$

These operators obey the commutation relations

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z, [\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x \text{ and } [\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y.$$

### orbital angular momentum quantum

**number** (B2: 53; B3: 10) For a *particle* or *spherically-symmetric system*, the orbital angular momentum quantum number is a non-negative integer,  $l$ , such that the possible values of the square of the magnitude of the orbital angular momentum are

$$L^2 = l(l+1)\hbar^2 \quad \text{where } l = 0, 1, 2, \dots$$

BOOK 3: The quantum number  $l$  can be used as a label for an *energy eigenfunction* in a *one-electron atom* or for an *atomic orbital* in the *central-field approximation*. When used in this way,  $l$  is restricted to the values  $0, 1, \dots, n-1$ , where  $n$  is the *principal quantum number* of the eigenfunction.

**order of a derivative** The number of times a function is differentiated. For example,  $d^3y/dx^3$  is a third-order derivative.

**order of a differential equation** (B1: 217) The highest *order of derivative* that appears in the *differential equation*.

**order of approximation** (B3: 79) If a quantity  $A$  depends on a small term  $\delta a$ , various approximations to  $A$  can be made. The *zeroth-order approximation* does not involve  $\delta a$ . The *first-order approximation* is equal to the zeroth-order approximation plus a correction that is proportional to  $\delta a$ . The *second-order approximation* is equal to the first-order approximation, plus a correction that is proportional to  $(\delta a)^2$ . In general, the  *$n$ th-order approximation* involves the terms up to, and including,  $(\delta a)^n$ , and the order of the approximation is said to be  $n$ . Do not confuse the  *$n$ th-order approximation* with the  *$n$ th-order correction*.

**ordinary differential equation** (B1: 217) A *differential equation* that involves only ordinary derivatives (and no *partial derivatives*). Sometimes, for brevity, called a differential equation.

**ordinary vector** (B2: 205) A physical quantity with a definite *magnitude* and direction in ordinary three-dimensional space. Often simply called a *vector*. Compare with *abstract vector*.

**orientation vector** (B2: 67) A *vector* used to specify the orientation of a *Stern–Gerlach magnet*. We arbitrarily choose this to point along the line of symmetry from the notched south pole piece to the pointed north pole piece, in the direction of increasing *magnetic field strength*.

**oriented area** (B2: 43) A *vector* quantity describing a planar surface, whose *magnitude* is equal to the area of the surface and whose direction is perpendicular to the surface. This gives two possible directions; the precise choice of direction may be made arbitrarily or may conform to a convention such as the *right-hand grip rule*.

**orthogonal functions** (B1: 102) Two functions  $f(x)$  and  $g(x)$  are said to be orthogonal if their *overlap integral* vanishes. That is,

$$\int_{-\infty}^{\infty} f^*(x) g(x) dx = 0.$$

This definition can be extended to three dimensions by taking the integral to be over all space.

BOOK 2: *Eigenfunctions* of a *linear Hermitian operator* are orthogonal if they correspond to different *eigenvalues*.

**orthogonal spin kets** Two *spin ket vectors*  $|A\rangle$  and  $|B\rangle$  are said to be orthogonal if their *inner product*  $\langle A|B\rangle$  is equal to zero. For example, spin kets corresponding to the *spin-up state* and the *spin-down state* in any given direction are orthogonal.

**orthogonal vectors** (B2: 17, 208) Two *vectors* are said to be orthogonal if their *inner product* vanishes. In ordinary space,  $\mathbf{a}$  is orthogonal to  $\mathbf{b}$  if  $\mathbf{a} \cdot \mathbf{b} = 0$ . In a *vector space*,  $|f\rangle$  is orthogonal to  $|g\rangle$  if  $\langle f|g\rangle = 0$ , in which case  $\langle g|f\rangle = 0$  too.

**orthonormal basis** (B2: 214) A *basis* in a *vector space* in which the *basis vectors* are *normalized* and mutually *orthogonal*.

**orthonormal set of functions** (B1: 103) A set of functions  $\psi_1(x), \psi_2(x), \dots$  is said to be orthonormal if each function is *normalized* and any pair of functions is *orthogonal*:

$$\int_{-\infty}^{\infty} \psi_i^*(x) \psi_j(x) dx = \delta_{ij},$$

where  $\delta_{ij}$  is the *Kronecker delta symbol*. This definition can be extended to three dimensions by taking the integral to be over all space.

**orthonormal set of vectors** (B2: 208) A set of *vectors*  $|\psi_1\rangle, |\psi_2\rangle, \dots$  is said to be orthonormal if each vector is *normalized* and any pair of vectors is *orthogonal*:

$$\langle \psi_i | \psi_j \rangle = \delta_{ij},$$

where  $\delta_{ij}$  is the *Kronecker delta symbol*.

**orthonormal spin kets** Two *spin ket vectors*  $|A\rangle$  and  $|B\rangle$  are said to be orthonormal if they are *normalized* ( $\langle A|A\rangle = \langle B|B\rangle = 1$ ) and mutually *orthogonal* ( $\langle A|B\rangle = \langle B|A\rangle = 0$ ).

**oscillation** A to-and-fro motion, also called a vibration.

**overlap integral** (B1: 101; B2: 11) In one dimension, the overlap integral of two functions  $f(x)$  and  $g(x)$  is given by

$$\int_{-\infty}^{\infty} f^*(x) g(x) dx.$$

This definition can be extended to three dimensions by taking the integral to be over all space. Overlap integrals are used to calculate *probability amplitudes* in *wave mechanics*.

BOOK 2: The overlap integral acts as the *inner product* for vectors  $|f\rangle$  and  $|g\rangle$  in *function space*.

**overlap rule** (B1: 101; B2: 132) For a one-dimensional system with discrete *non-degenerate energy eigenvalues*  $E_1, E_2, \dots$ , the overlap rule states that the *probability* of obtaining the  $i$ th *eigenvalue*  $E_i$  is

$$p_i = \left| \int_{-\infty}^{\infty} \psi_i^*(x) \Psi(x, t) dx \right|^2,$$

where  $\psi_i(x)$  is the *normalized energy eigenfunction* with eigenvalue  $E_i$ , and  $\Psi(x, t)$  is the *normalized wave function* describing the *state* of the system at the time of *measurement*. The integral between the *modulus* signs is called the *overlap integral* of  $\psi_i(x)$  and  $\Psi(x, t)$ .

This rule can be extended to other *observables* with discrete eigenvalues, provided that the energy eigenfunctions are replaced by the eigenfunctions of the corresponding quantum-mechanical *operator*.

BOOK 2: More generally, the overlap rule can be expressed using *Dirac notation*: for a system in a state described by the *state vector*  $|\Psi\rangle$ , the probability that a measurement of  $A$  will yield the result  $a_i$  is

$$p_i = |\langle a_i | \Psi \rangle|^2,$$

where  $|a_i\rangle$  is the *eigenvector* corresponding to the eigenvalue  $a_i$ . Provided the *inner product*  $\langle a_i | \Psi \rangle$  is interpreted appropriately, this form of the overlap rule applies to all systems, including those with *spin states*, three-dimensional systems and systems of many *particles*.

**p-type semiconductor** (B3: 191) A *semiconductor* that has been *doped* with a sufficient number of *acceptor atoms* for its electrical behaviour to be dominated by positively-charged *holes* in the *valence band*. Contrast with *n-type semiconductor*.

**pair production** (B3: 110) A process in which a *photon* can create an *electron-positron* pair. The photon must have *energy* greater than  $2m_e c^2$ , where  $m_e$  is the mass of an electron and  $c$  is the *speed of light* in a vacuum. Pair production requires the presence of an additional *particle* in order to conserve *energy* and *momentum*.

**parity** (B3: 22) In *Cartesian coordinates*, a function  $f(x, y, z)$  is said to have *even*

*parity* if  $f(-x, -y, -z) = f(x, y, z)$  for all  $x, y$  and  $z$ . It is said to have *odd parity* if  $f(-x, -y, -z) = -f(x, y, z)$ . In *spherical coordinates*, a function  $f(r, \theta, \phi)$  is said to have even parity if  $f(r, \pi - \theta, \pi + \phi) = f(r, \theta, \phi)$ . It is said to have odd parity if  $f(r, \pi - \theta, \pi + \phi) = -f(r, \theta, \phi)$ .

**Parseval's theorem** A term sometimes used in physics and engineering for *Plancherel's theorem*. Historically, Parseval proved a precursor of Plancherel's theorem for sums of *sinusoidal functions* (Fourier series) and it was Plancherel who proved the corresponding theorem for integrals (*Fourier transforms*).

**partial derivative** (B1: 222) The partial derivative  $\partial f / \partial x$  of a function  $f(x, y, \dots)$  with respect to the *independent variable*  $x$  is the derivative obtained by differentiating  $f$  with respect to  $x$  while treating all the other variables as constants.

**partial differential equation** (B1: 224) An equation that involves *partial derivatives* of an unknown function. See also *differential equation*.

**partial differentiation** The process of differentiating a function of two or more variables with respect to one of its variables, while treating all the other variables as constants.

**partial entanglement** See *partially entangled*.

**partially entangled** (B2: 154) In a *beam splitter*, a *state* is said to be partially entangled if the *probabilities* associated with the transmission or reflection of a *photon* are neither 0 and 1 (unentangled) nor 1/2 and 1/2 (fully-entangled).

**particle** (i) In the context of *classical physics*, a particle is an idealized object that is thought of as existing at a single point in space. It has no size, shape or internal motion though it may have intrinsic properties such as mass and *charge*, as well as position, velocity and acceleration.

(ii) In the context of high-energy physics, a particle is a piece of matter that is of sub-nuclear size (an *elementary particle*). Such particles include *protons*, *neutrons* and *electrons*, and may or may not be truly fundamental constituents of matter.

**particle decay** A general process whereby an unstable *elementary particle* can spontaneously change into two or more other elementary particles.

**particular solution** (B1: 218) A particular solution of a *differential equation* is a specific function that satisfies the equation and does not contain *arbitrary constants*. A particular solution is obtained from the *general solution* of the differential equation by choosing values for all the arbitrary constants. The choice is usually made by imposing additional physical restraints (*boundary conditions* or *initial conditions*).



**Pauli exclusion principle** (B2: 119) This principle stating that no two *identical fermions* can be in the same *quantum state* (i.e. they cannot have the same set of *quantum numbers*, including those for *spin*). Applied to *electrons*, the Pauli exclusion principle has profound consequences for the structure of *atoms*, *molecules* and solids, and is vital for an understanding of chemistry and the stability of matter.

**period** (B1: 17; B3: 128) (i) The time  $T$  taken for one complete *cycle* of an *oscillation* or *wave*; the reciprocal of the *frequency*:  $T = 1/f$ .

(ii) BOOK 3: The set of *elements* in a single row of the *Periodic Table*. Contrast with *group*.

**periodic boundary conditions** (B3: 179) *Boundary conditions* used in solid state physics. For a macroscopic cube of material, functions of interest (such as *energy eigenfunctions* or *wave functions*) are required to have the same values on opposite faces of the cube.

**Periodic Table** (B3: 128) A tabular arrangement of the chemical *elements*, ordered by *atomic number*  $Z$ , in which *shells* fill across horizontal rows called *periods*, and elements with similar patterns of *valence electrons*, and therefore similar chemical properties, appear in vertical columns called *groups*.

**periodicity of the lattice** (B3: 175) In a given *crystal*, a function  $f(\mathbf{r})$  is said to have the periodicity of the lattice if

$$f(\mathbf{r} + \mathbf{R}) = f(\mathbf{r})$$

for all *lattice vectors*  $\mathbf{R}$  joining points in the *lattice* of the crystal.

**permittivity of free space** (B1: 204) The fundamental constant  $\epsilon_0$  that appears in the proportionality factor  $1/4\pi\epsilon_0$  for *Coulomb's law* and hence determines the *magnitude* of the *electrostatic force* between two *electric charges* separated by a fixed distance in a vacuum. It also appears in the electrostatic *potential energy function* for two charges. In *SI units*,  $\epsilon_0 = 8.85 \times 10^{-12} \text{ F m}^{-1} = 8.85 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}$ , where  $\text{F}$  is the symbol for farad.

**perturbation** (B3: 77) A small contribution. In *quantum mechanics*, the small difference between a full *Hamiltonian* and a simplified *unperturbed Hamiltonian* is called a perturbation.

**perturbation method** (B3: 75) Another term for *perturbation theory*.

**perturbation theory** (B3: 75, 202) According to context, *time-independent perturbation theory* or *time-dependent perturbation theory*.

**perturbed Hamiltonian** (B3: 76) The *unperturbed Hamiltonian* plus the *perturbation*.

**phase** (B1: 18, 213) (i) For a *sinusoidal oscillation*  $x(t) = A \cos(\omega t + \phi)$ , where  $A$  is positive, the phase is the *argument* of the cosine, i.e.  $\omega t + \phi$ .

For a sinusoidal wave  $u(x, t) = A \cos(kx - \omega t + \phi)$ , where  $A$  is positive, the phase is the argument of the cosine, i.e.  $kx - \omega t + \phi$ . Do not confuse the phase with the *phase constant*.

(ii) For a *complex number* written in *polar* or *exponential form*:

$$z = r(\cos \theta + i \sin \theta) = r e^{i\theta},$$

the phase of the complex number is the *real number*  $\theta$  (also called the argument of the complex number).

(iii) The phase of a substance is a physically distinctive form of the substance that normally exists over a range of pressures and temperatures, such the solid, liquid and gas phases of water, or the magnetic or superconducting phases of a metal.

**phase constant** (B1: 18, 126) For a *sinusoidal oscillation*  $x(t) = A \cos(\omega t + \phi)$ , where  $A$  is positive, the phase constant is  $\phi$ .

For a sinusoidal wave  $u(x, t) = A \cos(kx - \omega t + \phi)$ , where  $A$  is positive, the phase constant is  $\phi$ . Do not confuse the phase constant with the *phase*.

**phase factor** (B1: 52, 214) A *complex number* of the form  $e^{i\alpha}$ , where  $\alpha$  is a *real number* called the *phase*. The *modulus* of a phase factor is equal to 1. Multiplying a *wave function* by an overall phase factor has no physical significance.

**photon** (B1: 10) A packet of *electromagnetic radiation*. For radiation in a vacuum, with *frequency*  $f$  and *angular frequency*  $\omega$ , each photon has *energy*  $E = hf = \hbar\omega$  and *momentum* of magnitude  $p = hf/c = \hbar\omega/c$ , where  $h$  is *Planck's constant*,  $\hbar$  is Planck's constant divided by  $2\pi$  and  $c$  is the *speed of light* in a vacuum. Photons are emitted and absorbed in *radiative transitions* between *energy levels*.

BOOK 2: A photon is a massless *boson* with *spin quantum number* 1. It has a *spin component* along its direction of motion of  $+\hbar$  for *left-handed circular polarization* and  $-\hbar$  for *right-handed circular polarization*.

**pion** (B3: 99) A class of *elementary particle*: positively-charged ( $\pi^+$ ) negatively-charged ( $\pi^-$ ) or neutral ( $\pi^0$ ). Charged pions have mass  $264m_e$ , and the neutral pions have mass  $273m_e$ , where  $m_e$  is the mass of an *electron*. Pions play an important role in the interaction between *protons* and *neutrons* at low *energies*. Pions contain *quark*–*antiquark* pairs. They are also known as  $\pi$ -mesons.

**plaintext** (B2: 180) An unencrypted message encoded as *bits*.

**Plancherel's theorem** (B1: 169) A mathematical

theorem stating that

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |A(k)|^2 dk,$$

where  $A(k)$  is the *Fourier transform* of  $f(x)$ . This theorem allows us to construct *normalized wave packets* for *free particles*, and underpins the interpretation of  $A(k)$  as a *momentum amplitude*. Plancherel's theorem is sometimes called *Parseval's theorem*.

**Planck distribution law** (B3: 217) A law stating that *electromagnetic radiation* in equilibrium with matter at an *absolute temperature*  $T$  has a *spectral energy density function*

$$u(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3} \frac{1}{e^{\hbar\omega/kT} - 1},$$

where  $\hbar$  is *Planck's constant* divided by  $2\pi$ ,  $c$  is the *speed of light* in a vacuum and  $k$  is *Boltzmann's constant*.

**Planck's constant** (B1: 10) The fundamental constant  $h = 6.63 \times 10^{-34}$  J s that appears in practically every equation of *quantum mechanics*, but never in those of *classical physics*. The quantity  $h/2\pi$  is given the symbol  $\hbar$ .

**plane wave** A wave of constant *frequency* for which points of constant *phase* lie in planes perpendicular to the direction of propagation of the wave.

**Poincaré sphere** (B2: 192) An abstract sphere used to parameterize the possible *quantum states* of a *qubit*. For the *polarization states* of a *photon*, the north pole of the Poincaré sphere represents a state of *vertical polarization*,  $|V\rangle$ , and the south pole represents a state of *horizontal polarization*,  $|H\rangle$ . All other points on the sphere correspond to states of polarization that are *linear superpositions* of  $|V\rangle$  and  $|H\rangle$ .

Points on the great circle that passes through the poles and intersects the  $x$ -axis correspond to states of *linear polarization*. The point where the sphere intersects the negative  $y$ -axis, corresponds to *right-handed circular polarization*, while the point where it intersects the positive  $y$ -axis, corresponds to *left-handed circular polarization*.

**polar angle** (B2: 49; B3:12) (i) In two dimensions, an angle of rotation about an axis perpendicular to the  $xy$ -plane, denoted by  $\theta$  and measured in radians. The polar angle lies in the range  $0 \leq \theta \leq 2\pi$ , and is measured anticlockwise from a value of zero along the positive  $x$ -axis. Along with the *radial coordinate*  $r$ , the polar angle  $\theta$  is of the *polar coordinates*.

(ii) In three dimensions, an angle of rotation around an axis in the  $xy$ -plane, denoted by  $\theta$  and measured in radians. The polar angle lies in the range  $0 \leq \theta \leq \pi$  and is equal to 0 along the positive  $z$ -axis,  $\pi/2$  in the  $xy$ -plane, and  $\pi$  along the negative  $z$ -axis. Along with

the radial coordinate  $r$  and the *azimuthal angle*  $\phi$ , the polar angle  $\theta$  is of the *spherical coordinates*.

**polar coordinates** (B2: 61) A pair of coordinates  $r$  and  $\theta$  used to specify the position of a point in a plane. Polar coordinates are related to two-dimensional *Cartesian coordinates*  $(x, y)$  by

$$x = r \cos \theta, \quad \text{and} \quad y = r \sin \theta.$$

The *radial coordinate* is given by  $r = \sqrt{x^2 + y^2}$  and the *polar angle*  $\theta$  is found by solving either  $\tan \theta = y/x$  or  $\cos \theta = x/r$  for  $\theta$ , taking care to choose an angle in the appropriate quadrant.

**polar form** (B1: 213) The polar form of a *complex number* is

$$z = r(\cos \theta + i \sin \theta),$$

where  $r$  is the *modulus* of the complex number and  $\theta$  is its *phase* or *argument*. The modulus lies in the range  $0 \leq r < \infty$ . It is always possible to add any integer multiple of  $2\pi$  to the phase without changing the complex number.

**polarization analyzer** (B2: 175) Another term for a *polarizing beam splitter*. Contrast with a *polarization preparer*.

**polarization preparer** A device that allows *photons* that are *linearly polarized* in one direction to be transmitted, while photons linearly polarized in the perpendicular direction are absorbed. A sheet of *Polaroid* functions in this way. Contrast with a *polarization analyzer*.

**polarization state** A partial specification of the *state* of a *photon* that refers only to polarization and omits all spatial or *frequency* information. A polarization state is represented by a *ket vector*. See also *linear polarization* and *circular polarization*.

**polarizing beam splitter** (B2: 168, 175) A *beam splitter* that sends a *photon* in one direction for one *state* of *linear polarization*, and in another direction for the perpendicular state of linear polarization. A photon in a general state of polarization will trigger detectors in one or other of the two output paths with *probabilities* that can be determined by *quantum mechanics*.

A polarizing beam splitter is the optical analogue of a *spin analyzer* and is sometimes called a *polarization analyzer*. See also *Wollaston prism*.

**Polaroid** The trademark name given to sheets of plastic, composed of aligned long-chain *molecules*, which absorb a high proportion of *light* that is *linearly polarized* in a given direction and transmit a high proportion of light that is linearly polarized in a perpendicular direction. Sheets of polaroid can be used as *polarization preparers*.

**position operator** (B1: 45) The quantum-mechanical *operator* representing the position of a *particle*. In one dimension, the position

operator is  $\hat{x} = x$ ; that is, the operation of multiplying a function  $f(x)$  by the variable  $x$ .

**BOOK 2:** The position operator  $\hat{x}$  is a *linear Hermitian operator*. It has no *eigenvalues*, and the possible values of position (all the *real numbers* times a unit of length) are given by its *generalized eigenvalues*.

**positional convention** (B2: 105) A convention used to specify the *spin ket* or *spin bra vector* of a *system* of two or more *particles*. For both bras and kets, the first entry refers to a particle with label 1, the second entry to a particle with label 2, and so on. For example,  $|\uparrow\downarrow\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2$  and  $\langle\uparrow\downarrow| = \langle\uparrow|_1 \langle\downarrow|_2$ .

**positron** (B3: 109) A positively-charged *elementary particle*, the *antiparticle* of an *electron*.

**positronium** (B3: 110) A short-lived *hydrogen-like system* consisting of an *electron* and a *positron* in a *bound state*.

**potential energy** *Energy* associated with the position of a *particle* or energy stored in a *system* by virtue of the positions of its component parts. In one dimension, a particle experiencing a conservative force  $F_x(x)$  has the *potential energy function*

$$V(x) = - \int F_x(x) dx + \text{constant}.$$

Equivalently,

$$F_x(x) = - \frac{dV}{dx}.$$

Any convenient point can be chosen to be the *zero of potential energy*.

**potential energy function** (B1: 46) A function describing the *potential energy* of a *particle* or *system*. Examples include the *free-particle* potential energy function which is a constant (usually taken to be zero) everywhere, the one-dimensional *harmonic oscillator* potential energy function  $V(x) = \frac{1}{2}Cx^2$ , and various *finite well* potential energy functions.

**potential energy operator** (B1: 45) The quantum-mechanical *operator* representing the *potential energy function* of a *system*. For a single *particle* in one dimension, the *potential energy operator* is  $\hat{V} = V(x)$ ; that is, the operation of multiplying a function  $f(x)$  by the potential energy function  $V(x)$ .

**principal quantum number** (B3: 46) A *quantum number*, denoted by  $n$ , that is used to label the *energy eigenfunctions* of the *electron* in a *one-electron atom* or the *atomic orbitals* of electrons in the *central-field approximation*. It can take integer values from 1 upwards. It is chiefly responsible for determining the *energy eigenvalue*. Solving the *time-independent Schrödinger equation* for the *Coulomb model* of a hydrogen atom leads to the energy eigenvalues  $E_n = -E_R/n^2$ , where  $E_R$  is the *Rydberg energy*.

**principle of superposition** (B1: 52, 219; B2: 110)

The property of a *linear homogeneous differential equation* whereby, if  $y_1(x)$  and  $y_2(x)$  are solutions of the differential equation, then so is the *linear combination*  $c_1y_1(x) + c_2y_2(x)$ , where  $c_1$  and  $c_2$  are any constants. *Schrödinger's equation* is a linear homogeneous *partial differential equation*, so the principle of superposition applies to it.

A version of the principle of superposition applies to *eigenvalue equations* for *linear operators*. If  $f(x)$  and  $g(x)$  are *eigenfunctions* of the linear operator  $\hat{A}$  with the same *eigenvalue*  $\lambda$  then, for any constants  $\alpha$  and  $\beta$ , the linear combination  $\alpha f(x) + \beta g(x)$  is also an eigenfunction of  $\hat{A}$  with eigenvalue  $\lambda$ .

**probabilistic** An alternative term for *indeterministic*.

**probability** (B1: 227) A number between 0 and 1 used to quantify the likelihood of an uncertain outcome, with larger probabilities corresponding to more likely outcomes; impossibility is represented by 0 and certainty by 1. See also the *addition rule for probability* and the *normalization rule*.

**probability amplitude** (B1: 31, 102) A quantity that emerges from quantum-mechanical calculations and refers to a given experimental outcome. The *probability* of a given outcome is obtained by taking the square of the *modulus* of the corresponding probability amplitude. Probability amplitudes can be calculated using the *overlap rule* or the *coefficient rule* and they are combined using the *interference rule*. Do not confuse a probability amplitude with the *amplitude* of a *wave* or *oscillation*.

**probability current** (B1: 190) A quantity that describes the rate of flow of *probability density* in one dimension. For a *particle* of mass  $m$ , or a beam of particles each of mass  $m$ , the probability current is defined by the relation

$$j_x(x, t) = -\frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right),$$

where  $\Psi(x, t)$  is the *wave function* describing the particle or beam. The probability current can be positive, negative or zero. The *SI* unit of probability current is  $\text{s}^{-1}$ . See also *beam intensity*.

**probability density** (B1: 50) For a *particle* in one dimension, in a *quantum state* described by the *wave function*  $\Psi(x, t)$ , the probability density is given by  $|\Psi(x, t)|^2$ . This is the *probability* per unit length of finding the particle in a small interval centred on  $x$ .

A similar definition applies in three dimensions, where the probability density  $|\Psi(\mathbf{r}, t)|^2$  is the probability per unit volume of finding the particle in a small region centred on  $\mathbf{r}$ .

Strictly speaking, the probability density is correctly called the *probability density function* for position.



**probability density function** (B1: 231) For any continuous *random* variable,  $a$ , the probability density function is a function  $\rho(a)$ , defined such that the *probability* of obtaining a value of  $a$  lying in a small range of width  $\delta a$ , centred on  $a_0$  is  $\rho(a_0) \delta a$ . The probability  $P$  of finding a value of  $a$  between  $a_1$  and  $a_2$  is

$$P = \int_{a_1}^{a_2} \rho(a) da.$$

The probability density function satisfies the *normalization condition*

$$\int_{-\infty}^{\infty} \rho(a) da = 1.$$

In *wave mechanics*, the probability density function for position is usually referred to simply as the *probability density*.

**probability distribution** (B1: 229) For a discrete *random* variable, a function that assigns a *probability* to each possible value of the variable. For a continuous random variable, a function that assigns a *probability density* to each possible value of the variable.

**protocol** (B2: 174) A convention that allows data transfer to take place.

**proton** An *elementary particle* which is a constituent of all atomic *nuclei*. The mass of a proton is slightly less than that of a *neutron* and is almost 2000 times greater than that of an *electron*. The *charge* of a proton is positive and has the same *magnitude* as that of a negatively-charged electron.

**proton–proton chain** (B1: 206) A sequence of nuclear reactions in stars like the Sun that have the net effect of converting *hydrogen* into *helium*.

**QED** An acronym for *quantum electrodynamics*.

**QKD** An acronym for *quantum key distribution*.

**quantization** (B1: 10) The phenomenon in which the measured values of some *observable* quantities have a discrete set of allowed values (in given *systems*, over given ranges).

**quantum communication channel** (B2: 181) A channel in which *quantum information* can be transported, generally encoded in the *states* of individual *photons*; it may use suitable optical fibre. Contrast with *classical communication channel*.

**quantum computing** (B2: 201) A field of study which attempts to construct computers whose logical operations rely on basic quantum-mechanical principles, especially the *principle of superposition*. See also *qubit*.

**quantum cryptography** (B2: 179) A field of study which uses basic quantum-mechanical principles to encode, transmit and decipher messages with

practically no risk of undetected eavesdropping. The methods used exploit the fact that a *measurement* irreversibly and uncontrollably changes the *state* of a *system*. *Entanglement* may, or may not, be used. See also *quantum key distribution*, the *BB84 protocol* and the *Eckert protocol*.

**quantum dot** (B1: 63; B3: 192) An artificially-created structure in which a tiny ‘speck’ of one *semiconducting material* is entirely embedded in a larger sample of another semiconducting material. The embedded speck is typically a few nanometres across. Such a structure can be modelled as a microscopic three-dimensional box in which *electrons* can be confined.

BOOK 3: The enclosed speck of semiconducting material has a smaller *band gap* than the surrounding host semiconductor. In the narrow band gap material, electrons at the bottom of the *conduction band* and *holes* at the top of the *valence band* have discrete *energy levels*. *Light* is emitted and *spectral lines* produced when electrons jump from the discrete electron levels in the conduction band to fill up the discrete hole levels in the valence band.

**quantum electrodynamics** (B3: 111) The sector of *quantum field theory* that relates to *electrons*, *positrons* and *photons*. It is a complete relativistic quantum field theory of the interaction between these *particles* and the *absorption* and *emission* of photons.

**quantum field theory** (B3: 111) The profound generalization of *quantum mechanics* that provides the framework for the full theory of atomic and subatomic *systems* with indefinite numbers of *particles*.

BOOK 3: See also *quantum electrodynamics*.

**quantum information** (B2: 201) A field of study in which the transformation and manipulation of information relies on basic quantum-mechanical principles. This field includes *quantum cryptography*, *quantum teleportation* and *quantum computing*.

**quantum key distribution** (B2: 181) The use of quantum-mechanical principles to transport *cryptographic keys* in such a way that any eavesdropping will be apparent to the users. The underlying principle is the fact that *measurements* irreversibly and unpredictably disturb the *system*.

**quantum measurement** (B2: 136) See *measurement*.

**quantum mechanics** (B1: 7) The comprehensive quantum theory of *systems* of finite numbers of *particles* that superseded *old quantum theory* and *classical mechanics*. Quantum mechanics has both non-relativistic and relativistic branches, but it does not cover systems in which particles are created or destroyed: that is the province of *quantum field theory*. This course focuses mainly on the non-relativistic aspects of quantum mechanics.

**quantum number** (B1: 57) A discrete index (often, but not always, an integer) used to label discrete *eigenvalues*, *eigenfunctions*, *stationary state wave functions* or *quantum states* in a given system. For example, a *particle* in a *one-dimensional infinite square well* has *energy eigenvalues* labelled by a positive integer  $n$ ..

A single quantum number is enough to specify the quantum state of a spinless particle in a one-dimension. At least three quantum numbers are needed to fully specify a state in a three-dimensional system.

**quantum physics** (B1: 7) A term given to any branch of physics that is based on quantum ideas. For example, aspects of nuclear physics, atomic physics or *quantum field theory* may be classified as being quantum physics.

**quantum random number generator** (B1: 15) A device that uses the fundamental *probabilistic* nature of *quantum mechanics* to generate a sequence of *random numbers*.

**quantum state** A specified *state* of a *quantum system*. *Quantum mechanics* is *indeterministic*, so precise knowledge of the quantum state of a system may not allow us to predict with certainty the results of all *measurements* taken on the system.

**quantum system** A *system* that is analyzed according to the principles of *quantum physics*, rather than *classical physics*. Since quantum physics is assumed to be universally valid, any system might be taken to be a quantum system; in practice, macroscopic systems are often taken treated classically without discernible error.

**quantum teleportation** (B2: 193) The use of quantum-mechanical methods to copy the unknown *quantum state* of a *system* to a distant location. For *photons*, teleportation of the unknown *polarization state* of photon 1 can be achieved with the aid an *entangled* pair of photons, 2 and 3. Photon 3 is sent to a distant location and photon 2 is sent through a *beam splitter* in conjunction with photon 1, from which it is *indistinguishable*. A *Bell state measurement* on photons 1 and 2 causes photon 3 to collapse into a state that is simply related to the unknown initial state of photon 1.

Depending on the result of the Bell state measurement (there are four possibilities) a message sent over a *classical communication channel* will provide the information needed to convert the state of photon 3 into the unknown initial state photon 1. After the Bell state measurement the initial state of photon 1 is destroyed, so quantum teleportation does not contravene the *no-cloning theorem*.

**quantum wafer** (B1: 64) An artificially-created structure in which a thin layer of one *semiconducting*

*material* is sandwiched between thicker layers of another semiconducting material. The thin layer is typically a few nanometres thick. Such a structure allows *electrons* to move freely in two dimensions while being narrowly confined in the third.

**quantum wire** (B1: 63) An artificially-created structure in which a thin ‘thread’ of one *semiconducting material* is embedded in another semiconducting material. The embedded thread is typically a few nanometres across. Such a structure allows *electrons* to move freely in one dimension while being narrowly confined in the other two dimensions.

**quark** (B3: 112) Any of the charged *elementary particles* that are currently believed to be fundamental constituents of *protons*, *neutrons*, *pions* and other sub-atomic particles (collectively known as hadrons). Six kinds of quark are currently known: up, down, charm, strange, top and bottom. Quarks are not expected to be observed as isolated particles.

All quarks have *spin*- $\frac{1}{2}$  and an *electric charge* that is a multiple of  $\frac{1}{3}e$ . A proton consists of three quarks, two with charge  $+\frac{2}{3}e$  and one with charge  $-\frac{1}{3}e$ , plus gluons that bind them together. A neutron consists of three quarks, two with charge  $-\frac{1}{3}e$  and one with charge  $+\frac{2}{3}e$ , plus gluons.

**quarkonium** (B3: 112) Short-lived *bound states* of a heavy *quark* and an antiquark that can be created in collisions between *elementary particles* in large accelerators.

**qubit** (B2: 192) A quantum bit, the counterpart in *quantum computing* to the binary digit or *bit* of classical computing. A qubit is specified by the *quantum state* of a *system* whose states are represented by *vectors* in a two-dimensional *vector space* with two *orthonormal basis vectors*  $|0\rangle$  and  $|1\rangle$ . The qubit is represented by any *normalized linear combination* of  $|0\rangle$  and  $|1\rangle$ , such as  $c_0|0\rangle + c_1|1\rangle$  with  $|c_0|^2 + |c_1|^2 = 1$ , and therefore contains far more information than a classical bit.

**radial coordinate** (B2: 49; B3: 12) The distance, denoted by  $r$ , of a point from the origin. This is one of the *polar coordinates* in two dimensions and one of the *spherical coordinates* in three dimensions.

**radial equation** (B3: 40) In the context of finding the *energy eigenfunctions* of a *one-electron atom* or an *atom* in the *central-field approximation*, this is a *differential equation* dependent only on  $r$ , which is obtained by separating the  $r$ -dependence from the  $\theta$ - and  $\phi$ -dependences in the *time-independent Schrödinger equation* for the atom.

**radial function** (B3: 40) A solution,  $R_{nl}(r)$ , of the *radial equation* for a *one-electron atom* or an *atom* in the *central-field approximation*. The radial

function describes the dependence of an *energy eigenfunction* for the atom on the *radial coordinate*. In a given *system*, each radial function is labelled by the *principal quantum number*  $n$  and the *orbital angular momentum quantum number*  $l$ .

**radial probability density** (B3: 55) The *probability* per unit radial distance of finding a *particle* at radial distance  $r$  from the origin. For a *hydrogen atom*, the radial probability density is the probability per unit radial distance that the *electron–proton* separation is  $r$ ; this is given by  $R_{nl}^2(r) r^2$ , where  $R_{nl}(r)$  is the *radial function*. The probability that the electron–proton separation is between  $r$  and  $r + \delta r$  is  $R_{nl}^2(r) r^2 \delta r$ .

**radiative transition** (B1: 145; B3: 197) A process in which a *system* (such as an *atom*) undergoes a transition from one *quantum state* to another by the emission or absorption of *electromagnetic radiation*. Such a process involves the creation or destruction of a *photon* (or, very rarely, more than one photon). BOOK 3: There are three types of radiative transition: *absorption*, *stimulated emission* and *spontaneous emission*.

**radioactive decay** A process in which an unstable *nucleus* loses *energy* by emitting ionizing *particles* and *electromagnetic radiation* and, as a result, transforms into a different type of nucleus.

**raising operator** (B1: 137) For a *harmonic oscillator* with *length parameter*  $a$ , the raising operator is defined as

$$\hat{A}^\dagger = \frac{1}{\sqrt{2}} \left( \frac{x}{a} - a \frac{\partial}{\partial x} \right),$$

This operator converts an *energy eigenfunction*  $\psi_n(x)$  of the oscillator into the next eigenfunction of higher energy. If the eigenfunctions are *normalized*,

$$\hat{A}^\dagger \psi_n(x) = \sqrt{n+1} \psi_{n+1}(x).$$

for  $n = 0, 1, 2, \dots$ . See also *lowering operator* and *ladder operator*.

**Ramsauer–Townsend effect** (B1: 196) A sharp dip in the measured *total cross-section* for the *scattering* of *electrons* by *noble gas atoms* (such as xenon) at an *energy* of about 1 eV. This is a three-dimensional analogue of the *transmission resonance* found in one dimension.

**random** (B1: 227) A variable is said to be random if its possible values have definite *probabilities*, but no further information is available to us about which of its values will be obtained.

**real axis** (B1: 212) An axis in the *complex plane* on which *complex numbers* have zero *imaginary part* and which points in the direction of increasing *real part*.

**real number** An ordinary number; in other words, a *complex number* with no *imaginary part*.

**real part** (B1: 210) Given a *complex number*  $z = x + iy$ , where  $x$  and  $y$  are *real numbers*, the real part of  $z$  is equal to  $x$ . The real part of any complex expression is given by

$$\text{Re}(z) = \frac{z + z^*}{2},$$

where  $z^*$  is the *complex conjugate* of  $z$ .

**realism** (B2: 161) The assertion that *observable* quantities always have definite values, whether or not these values have been determined by *measurement*. Realism is not consistent with *quantum mechanics*, but it is a key feature of *hidden-variable theories*.

**reduced mass** (B1: 128; B3: 37) A mass used to characterize a two-particle *system*. If the two *particles* have masses  $m_1$  and  $m_2$ , the reduced mass of the two-particle system is

$$\mu = \frac{m_1 m_2}{m_1 + m_2}.$$

For two particles with positions  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , interacting via a mutual *potential energy function*  $V(\mathbf{r}_2 - \mathbf{r}_1)$ , the relative position  $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$  obeys the same equations as a single particle of mass  $\mu$  in a potential energy well  $V(\mathbf{r})$ .

The reduced mass is always smaller than the mass of either of the particles in the system. In a *hydrogen atom*,  $\mu$  is 0.9995 the mass of an *electron*, but for a *diatomic molecule* composed of two similar *atoms*, it is half the mass of either atom.

**reduced radial equation** (B3: 40) For a *one-electron atom* or other *atom* in the *central-field approximation*, the reduced radial equation is a *differential equation* for the *reduced radial function*  $u(r)$ , obtained from the *radial equation* by replacing the *radial function*  $R(r)$  by  $u(r)/r$ , where  $r$  is the *radial coordinate*.

**reduced radial function** (B3: 40) The function  $u(r) = rR(r)$ , where  $R(r)$  is the *radial function* for a *one-electron atom* or other *atom* in the *central-field approximation*, and  $r$  is the *radial coordinate*.

**reflection coefficient** (B1: 182) The *probability* that a specified one-dimensional *potential energy function* will cause an incident *particle* to reverse its direction of motion. Compare with *transmission coefficient*.

**relative atomic mass** (B3: 101) The mass of an *atom* in units of one-twelfth of the mass of a carbon-12 atom. This is quite close to the *mass number*, which is the total number of *protons* and *neutrons* in the *nucleus* of the atom.

**relative frequency** (B1: 229) If a quantity  $A$  is measured  $N$  times and the result  $A_i$  is obtained on  $N_i$  occasions, the relative frequency of the result  $A_i$  is  $N_i/N$ . In the long run, this relative frequency is expected to tend to the corresponding *probability*,  $p_i$ .



**relaxation time** (B3: 188) In the context of electrical conduction, the average time an *electron* spends between collisions.

**restoring force** (B1: 125) A force that acts in a direction which tends to restore a *particle* towards its equilibrium position.

**right-hand grip rule** (B2: 43) A rule used to determine the direction of the *magnetic dipole moment* of a *current* loop. With the curled fingers of your right hand wrapped around the loop in the direction of current flow, your outstretched right thumb indicates the direction of the magnetic dipole moment, perpendicular to the plane of the current loop.

**right-hand rule** (B2: 40, 209) A rule used to determine the direction of a *vector product*  $\mathbf{a} \times \mathbf{b}$ : point your right hand in the direction of the first *vector*,  $\mathbf{a}$ , and bend your fingers to point in the direction of the second vector,  $\mathbf{b}$ . The vector product  $\mathbf{a} \times \mathbf{b}$  is perpendicular to both  $\mathbf{a}$  and  $\mathbf{b}$ , in the direction of your outstretched right thumb.

**right-handed circular polarization** See *circular polarization*.

**row matrix** (B2: 215) A *matrix* with a single row.

**row spinor** (B2: 78) A *row matrix* used to represent a *spin bra vector*.

**Rydberg energy** (B3: 37) The *energy*  $E_R$  required to cause the *ionization* of a *hydrogen atom* from its *ground state*. The solution of the *time-independent Schrödinger equation* predicts that

$$E_R = \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{\mu}{2\hbar^2} = 13.6 \text{ eV},$$

where  $\mu$  is the *reduced mass* of the *electron* and *proton* in the atom, and this is in good agreement with experimental data. The *Bohr model* makes a similar prediction.

**Rydberg states** (B3: 60) *Quantum states* of an *atom* with very high values of the *principal quantum number*,  $n$ .

**sandwich integral** (B1: 112) An integral of the form

$$\int_{-\infty}^{\infty} \Psi^*(x, t) \hat{A} \Psi(x, t) dx,$$

used in the *sandwich integral rule*.

**sandwich integral rule** (B1: 112) In a *quantum state* described by the *wave function*  $\Psi(x, t)$ , the *expectation value* of an *observable*  $A$  is given by the *sandwich integral*

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{A} \Psi(x, t) dx,$$

where  $\hat{A}$  is the quantum-mechanical *operator* corresponding to  $A$ .

**BOOK 2:** In *Dirac notation*, the sandwich integral rule becomes the *sandwich rule*.

**sandwich rule** (B2: 89, 134) In the *quantum state* represented by *state vector*  $|\Psi\rangle$ , the *expectation value* of the *observable*  $A$  is given by

$$\langle A \rangle = \langle \Psi | \hat{A} | \Psi \rangle \equiv \langle \Psi | \hat{A} \Psi \rangle,$$

where  $\hat{A}$  is the quantum-mechanical *operator* corresponding to  $A$ . Special cases are the *sandwich integral rule* and the *sandwich rule for spin*.

**sandwich rule for spin** (B2: 89) A special case of the *sandwich rule* which states that the *expectation value* of a *spin observable*  $S$  in a *spin state*  $|A\rangle$  is given by

$$\langle S \rangle = \langle A | \hat{S} | A \rangle,$$

where  $\hat{S}$  is the quantum-mechanical *operator* corresponding to  $S$ . For a *spin- $\frac{1}{2}$  particle*,  $\hat{S}$  is a  $2 \times 2$  *square matrix*,  $|A\rangle$  is a  $2 \times 1$  *column spinor* and  $\langle A|$  is a  $1 \times 2$  *row spinor*.

**scalar** (B2: 205) A quantity that is completely specified by a single number, or by a number times an appropriate unit of measurement. Contrast with *vector*.

**scalar product** (B2: 12, 207) For two *ordinary vectors*  $\mathbf{a}$  and  $\mathbf{b}$ , the scalar product is a *scalar* quantity defined by

$$\begin{aligned} \mathbf{a} \cdot \mathbf{b} &= a_1 b_1 + a_2 b_2 + a_3 b_3 \\ &= ab \cos \theta, \end{aligned}$$

where the vectors have *components*  $a_i$  and  $b_i$  and *magnitudes*  $a$  and  $b$ . The angle  $\theta$  is the angle between the directions of the vectors taken to be in the range  $0 \leq \theta \leq \pi$ . The scalar product is an *inner product* for ordinary space.

**scaled Bohr radius** (B3: 92) For a *hydrogen-like atom* with *atomic number*  $Z$ , the scaled Bohr radius is

$$a_0^{\text{scaled}} = \frac{1}{Z} \frac{\mu_H}{\mu} a_0,$$

where  $\mu$  is the *reduced mass* of the hydrogen-like atom,  $\mu_H$  is the reduced mass of a *hydrogen atom* and  $a_0$  is the *Bohr radius*. The scaled Bohr radius sets the scale for the spatial extent of the *radial function* in any hydrogen-like atom.

**scaled Rydberg energy** (B3: 92) For a *hydrogen-like atom* with *atomic number*  $Z$ , the scaled Rydberg energy is

$$E_R^{\text{scaled}} = Z^2 \frac{\mu}{\mu_H} E_R,$$

where  $\mu$  is the *reduced mass* of the hydrogen-like atom,  $\mu_H$  is the reduced mass of a *hydrogen atom* and  $E_R$  is the *Rydberg energy*. The scaled Rydberg energy sets the scale for the *energy eigenvalues* in any hydrogen-like atom.

**scanning tunnelling microscope** (B1: 206) A type of microscope that produces atomic-scale maps of surface structure by monitoring the *tunnelling* of *electrons* through the tiny gap between a sample's surface and a very narrow probe tip that is scanned across the surface.

**scattering** (B1: 178) A process in which an incident *particle* or *wave* is affected by interaction with some kind of target, quite possibly another particle. The interaction can affect the incident particle in a number of ways; it may change its *kinetic energy*, direction of motion or *quantum state* of internal excitation. Particles can even be created, destroyed or absorbed. Scattering may be *elastic* or *inelastic*.

In one dimension, scattering can be described in terms of the *reflection coefficient* and the *transmission coefficient*. More generally, it is described in terms of the *total cross-section* and the *differential cross-section*.

**Schrödinger cat paradox** (B2: 140) A thought experiment invented by Schrödinger in which a cat is placed in a closed box containing a lethal device that can be triggered by an unlikely quantum event. According to conventional *quantum mechanics*, prior to a *measurement*, the cat is in a *linear superposition* of two *quantum states* — one in which it is dead and another in which it is alive. Only on opening the box and ‘making a measurement’ do we cause the cat’s *state vector* to undergo to collapse onto either a living cat or a dead cat.

**Schrödinger’s equation** (B1: 24, 46) The *partial differential equation* that governs the time development of the *wave function*  $\Psi$  describing the *state* of a *system* in *wave mechanics*. Schrödinger’s equation can be written in the general form

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi,$$

where  $\hat{H}$  is the *Hamiltonian operator* of the system and  $\hbar$  is *Planck’s constant* divided by  $2\pi$ .

In any specific situation  $\hat{H}$  takes a form that characterizes the system under consideration, and  $\Psi$  depends on the possible coordinates of *particles* in the system as well as on time. For example, in the case of a one-dimensional system consisting of a particle with *potential energy function*  $V(x)$ , Schrödinger’s equation takes the form

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x)\Psi(x, t).$$

BOOK 2: In *Dirac notation*, Schrödinger’s equation takes the general form

$$i\hbar \frac{d|\Psi\rangle}{dt} = \hat{H}|\Psi\rangle.$$

and this equation applies to the time-evolution of *spin states* as well that of *spatial wave functions*.

**screening** (B3: 125) In atomic physics, screening refers to a physical effect by which the attraction felt by an *electron* towards the *nucleus* is partially or totally compensated by repulsion caused by other electrons in the *atom*. This can be represented by a reduction in the effective nuclear *charge*.

**second-order approximation** See *order of approximation*.

**second-order correction** (B3: 80) In *perturbation theory*, the second-order correction is the additional term, proportional to the square of the *perturbation*, that must be added to the *first-order approximation* to produce the *second-order approximation*.

**second-order partial derivative** (B1: 224) A function obtained by partially differentiating another function twice (possibly with respect to different *independent variables*).

**secular determinant** (B3: 151) A *determinant* obtained using the *LCAO approximation* and the *variational method* in the course of finding approximate *electronic energies* in *molecules* and *solids*. This determinant appears in the *secular equation*.

**secular equation** (B3: 151) An equation that emerges from applying the *LCAO approximation* and the *variational method* to *molecules* and *solids*. The equation is a condition that must be satisfied in order for the *trial function*  $\psi$  to provide an extremum for  $\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$ , the *expectation value* of the *energy*. It takes the form of a polynomial equation for  $\langle E \rangle$ , and its roots provide approximations for *electronic energies* in the molecule or solid.

**selection rules** (B1: 131; B3: 208) Rules that govern whether particular *radiative transitions* are allowed or (to a first approximation at least) forbidden. In a *harmonic oscillator*, for example, a selection rule restricts radiative transitions to those between neighbouring *energy levels*.

BOOK 3: In practice, selection rules allow only the radiative transitions that occur within the *electric dipole approximation* and first-order *time-dependent perturbation theory*. It may be possible for other radiative transitions to occur, but these are very much weaker and may go undetected. For a *one-electron atom* or other *atoms* within the *central-field approximation*, the selection rules for the *orbital angular momentum quantum number* and the *magnetic quantum number* are  $\Delta l = \pm 1$  and  $\Delta m = 0$  or  $\pm 1$ .

**self-consistency** (B3: 126) In the context of atomic physics, self-consistency refers to the choice of a *potential energy function* that is consistent with the distribution of electronic *charge* obtained by solving the *time-independent Schrödinger equation* for a

given *atom*. Self-consistency is generally reached by an iterative procedure.

**semiconducting material** (B1: 63) A material with an *electrical conductivity* intermediate between those of *conductors* and *insulators*. Examples include silicon and germanium. BOOK 3: See also *semiconductor*.

**semiconductor** (B3: 187) A material with a gap between the *valence band* and the *conduction band*, but which nevertheless conducts electricity quite well with an *electrical conductivity* intermediate between those of *conductors* and *insulators*. This may be because the *band gap* is small or because the material incorporates sufficient numbers of *donor atoms* or *acceptor atoms*. The band gap of a pure semiconductor is less than about  $80kT$  at *absolute temperature*  $T$ , where  $k$  is *Boltzmann's constant*; this corresponds to a band gap smaller than about 2 eV at room temperature. Contrast with *conductor* and *insulator*.

**separable partial differential equation** (B1: 226) A *partial differential equation* for which the method of *separation of variables* can be applied successfully. Special solutions of the partial differential equation can then be found which are products of single-variable functions of all the *independent variables* in the equation.

**separation constant** (B1: 54, 226) An undetermined constant that appears when a *partial differential equation* is solved by the method of *separation of variables*. The separation constant then appears in the *eigenvalue equations* for the separated variables.

**separation of variables** (B1: 53, 225) A method used for finding some solutions of some *partial differential equations*. It involves looking for solutions that are products  $X(x)Y(y)\dots$  of single-variable functions of each *independent variable* in the equation. Substituting a solution of this form into the partial differential equation and rearranging terms leads to an equation in which one variable appears only on the left-hand side and the others appear only on the right. Each side of the equation can then be equated to the same *separation constant*. This procedure is repeated for the remaining variables until each of the functions  $X(x)$ ,  $Y(y)$  appears in its own *ordinary differential equation*. Multiplying the solutions of these ordinary differential equations together gives special solutions of the original partial differential equation.

In the case of *Schrödinger's equation* for a one-dimensional system consisting of a *particle* with a given *potential energy function*  $V(x)$  that is independent of time, a product solution takes the form  $\psi(x)T(t)$ , where  $\psi(x)$  is a solution of the *time-independent Schrödinger equation* for the

system,  $T(t) = e^{-iEt/\hbar}$ , and the separation constant  $E$  represents the total *energy* of the system.

**shell** (B3: 126) In the *central-field approximation* of an *atom*, a shell is a collection of *atomic orbitals* that share the same *principal quantum number*  $n$  and *orbital angular momentum quantum number*,  $l$ . See also *closed shell* and *open shell*.

**SI** An internationally agreed system of units of measurement. The system employs seven base units, including the kilogram (abbreviated to kg), the metre (abbreviated to m), the second (abbreviated to s), the ampere (abbreviated to A) and the *kelvin* (abbreviated to K). It also includes a number of derived units obtained by combining base units in various ways.

The SI system uses certain standard prefixes such as kilo =  $10^3$ , mega =  $10^6$ , giga =  $10^9$ , tera =  $10^{12}$ , milli =  $10^{-3}$ , micro =  $10^{-6}$ , nano =  $10^{-9}$  and pico =  $10^{-12}$ . It also recognizes a number of standard symbols and abbreviations. SI itself is one of these symbols and stands for *Système International*.

**simple harmonic motion** (B1: 124) In *classical physics*, a particular type of *oscillation* of a *particle* about a specified equilibrium position, characterized by the fact that the acceleration of the particle is always directed towards the equilibrium position and is proportional to the displacement from that point. In one dimension, simple harmonic motion may be described by a *differential equation* of the form

$$\frac{d^2x}{dt^2} + \omega_0^2 x = 0,$$

which has the *general solution*

$$x(t) = A \cos(\omega_0 t + \phi),$$

where  $A$  is the *amplitude* of the motion,  $\omega_0$  is the *angular frequency* and  $\phi$  is the *phase constant* of the motion.

**simple harmonic oscillation** Another term for *simple harmonic motion*.

**simple harmonic oscillator** In *classical physics*, a *particle* or *system* that performs *simple harmonic motion*. Another term for a *harmonic oscillator*.

**single bond** (B3: 163) In the *LCAO approximation* for *molecules*, a chemical bond with a *formal bond order* of 1 is referred to as a single bond.

**single-valuedness condition** (B2: 51) The condition that requires that a function  $f(\phi)$ , where  $\phi$  represents an angle measured in radians, should return to the same value when  $\phi$  changes by  $2\pi$ . Applied to the *eigenfunctions* of the *angular momentum operator*  $\hat{L}_z$ , this condition leads to the *quantization* of  $L_z$ .

**singlet state** (B2: 114) The *spin state* of a system of two *spin- $\frac{1}{2}$  particles* for which the *total spin quantum number* is  $S = 0$ . This state is *antisymmetric* with respect to exchange of the particle labels. Compare with *triplet state*.



**sinusoidal** Any function of the form

$$f(x) = A \sin(kx + \phi)$$

where  $A$ ,  $k$  and  $\phi$  are *real* constants, may be described as a sinusoidal function. Thus any *linear combination* of  $\sin x$  and  $\cos x$ , with real coefficients, is a sinusoidal function.

**span** (B2: 12, 17) A set of *vectors* is said to span a *vector space* if any vector in the space can be expressed as a *linear combination* of the vectors from the set. We may also say that the vectors form a *complete set* or *basis* for the vector space.

**spatial wave function** (B2: 105) A partial specification of the *state* of a *system* given by a *wave function* that depends only on the spatial coordinates of the *particles* in the system and therefore describes the spatial part of the *total wave function*. Compare with *spin ket vector*.

**spectra** The plural of *spectrum*.

**spectral energy density function** (B3: 214) A function  $u(\omega)$  defined such that  $u(\omega) \delta\omega$  is the *energy density* of *electromagnetic radiation* contributed by *angular frequencies* in a small range of width  $\delta\omega$ , centred on  $\omega$ .

**spectral lines** (B1: 9) Narrow lines (corresponding to narrow ranges of *frequency* or *wavelength*) seen in the *spectra* of substances and characteristic of those substances. Each spectral line results from a *radiative transition* and has a frequency  $f = \Delta E/h$ , where  $\Delta E$  is the *magnitude* of the *energy* difference between the initial and final *quantum states* and  $h$  is *Planck's constant*.

**spectroscopic dissociation energy** (B3: 155) For a *diatomic molecule* in a given *electronic state*, the spectroscopic dissociation energy is the *magnitude* of the difference between the minimum *energy* of the *energy curve* and the energy that corresponds to two separated *atoms*. In the *electronic ground state*, the spectroscopic dissociation energy exceeds the directly-measured *dissociation energy* by the vibrational *zero-point energy* of the *nuclei*.

**spectroscopic notation** See individual entries for *spectroscopic notation for atomic orbitals*, *spectroscopic notation for atomic terms*, *spectroscopic notation for atomic levels* and *spectroscopic notation for molecular orbitals*.

**spectroscopic notation for atomic levels** (B3: 137) A particular *atomic level* is denoted by the spectroscopic symbol

$$^{2S+1}L_J,$$

where  $L$  is equal to S, P, D, F, ... for  $L = 0, 1, 2, 3, \dots$ . Here,  $L$  is the *total orbital angular momentum quantum number*,  $S$  is the *total*

*spin quantum number* and  $J$  is the *total angular momentum quantum number*.

**spectroscopic notation for atomic orbitals** (B3: 117) A method of labelling *atomic orbitals* and *energy levels* with a letter that denotes the value of the *orbital angular momentum quantum number*  $l$ . Orbitals with  $l = 0$  are labelled s, those with  $l = 1$  are labelled p, those with  $l = 2$  are labelled d, and those with  $l = 3$  are labelled f. Orbitals with higher values of  $l$  are labelled alphabetically starting from g for  $l = 4$ . The letters are prefixed by the value of the *principal quantum number*  $n$ , and a subscript can be added to indicate the value of the *magnetic quantum number*  $m$ . Thus an orbital with  $n = 3$ ,  $l = 1$  and  $m = 0$  is denoted  $3p_0$ , and an orbital with  $n = 5$ ,  $l = 4$  and  $m = -3$  is denoted  $5g_{-3}$ .

**spectroscopic notation for atomic terms** (B3: 135) A particular *atomic term* is denoted by the spectroscopic symbol

$$^{2S+1}L,$$

where  $L$  is equal to S, P, D, F, ... for  $L = 0, 1, 2, 3, \dots$ . Here,  $L$  is the *total orbital angular momentum quantum number*,  $S$  is the *total spin quantum number* and  $2S + 1$  is called the *multiplicity* of the atomic term.

**spectroscopic notation for molecular orbitals** (B3: 157) A method of labelling the *molecular orbitals* of *diatomic molecules* according to the value of  $|m|$ , where  $m$  is the *magnetic quantum number* of the molecular orbital. Orbitals with  $|m| = 0$  are labelled  $\sigma$ ; those with  $|m| = 1$  are labelled  $\pi$ , and so on. Orbitals of *homonuclear diatomic molecules* have a subscript g (for *even parity*) or u (for *odd parity*). The lower case Greek letter is prefaced by a number, which orders molecular orbitals of the same type by increasing *energy*.

**spectrum** (B1: 9) Any particular distribution of *electromagnetic radiation*, expressed as a function of *intensity* versus *wavelength*, *frequency* or a related quantity such as *photon energy*. Many spectra consist of *spectral lines*, produced during *radiative transitions* between discrete *quantum states*. Such a spectrum can provide an identifiable 'fingerprint' of a substance. BOOK 3: By contrast, a continuous spectrum, is a continuous distribution of intensity produced in processes such as *bremsstrahlung*.

**speed of light** The speed of an *electromagnetic wave*. In an *inertial frame of reference*, in a vacuum, this is a universal constant  $c = 3.00 \times 10^8 \text{ m s}^{-1}$ , independent of *amplitude*, *frequency*, *wavelength* or motion of the source.

**spherical coordinates** (B2: 49; B3: 12) Coordinates  $r$ ,  $\theta$  and  $\phi$ , used to define the position of a point in three-dimensional space, where  $0 \leq r < \infty$  is the

radial coordinate,  $0 \leq \theta \leq \pi$  is the polar angle and  $0 \leq \phi \leq 2\pi$  is the azimuthal angle.

Spherical coordinates are related to the Cartesian coordinates  $x$ ,  $y$  and  $z$  by

$$\begin{aligned}x &= r \sin \theta \cos \phi, \\y &= r \sin \theta \sin \phi, \\z &= r \cos \theta,\end{aligned}$$

which is consistent with  $r = \sqrt{x^2 + y^2 + z^2}$ .

**spherical harmonics** (B3: 18) Finite and single-valued functions  $Y_{lm}(\theta, \phi)$  of the spherical coordinates  $\theta$  and  $\phi$  that are simultaneous eigenfunctions of  $\hat{L}^2$  and  $\hat{L}_z$  (the operators for the square of the magnitude of, and the  $z$ -component of, the orbital angular momentum).

The spherical harmonic  $Y_{lm}(\theta, \phi)$  is an eigenfunction of  $\hat{L}^2$  with eigenvalue  $l(l+1)\hbar^2$ , where  $l = 0, 1, 2, \dots$  is the orbital angular momentum quantum number. It is simultaneously an eigenfunction of  $\hat{L}_z$  with eigenvalue  $m\hbar$ , where  $m = -l, -l+1, \dots, l-1, l$  is the magnetic quantum number. In general,  $Y_{lm}$  involves powers of  $\sin \theta$  and  $\cos \theta$  and is proportional to  $e^{im\phi}$ . It has parity  $(-1)^l$ .

**spherically-symmetric** (B3: 12) A quantity  $f$  is spherically-symmetric about the origin if it depends only on the distance from the origin. In spherical coordinates, this allows us to write  $f(r)$  rather than  $f(r, \theta, \phi)$ .

Considered as a whole, and viewed from a fixed external frame of reference, an isolated system such as a diatomic molecule may be regarded as being spherically-symmetric because its Hamiltonian operator keeps the same form when the coordinate system is rotated about any axis (for example, the terms describing the various potential energies remain unchanged because they depend only on the distances between particles, and these distances are unchanged by rotation).

**spin** (B2: 67) See spin angular momentum.

**spin analyzer** (B2: 69) A Stern–Gerlach apparatus in which both of the sub-beams leaving the magnetic field region are detected. Contrast with spin preparer.

**spin angular momentum** (B2: 40, 67) A type of angular momentum possessed by elementary particles such as electrons and protons, and by composite particles such as atoms and nuclei irrespective of their motion through space. Particles with a spin quantum number  $s = \frac{1}{2}$  have two possible values of any component of spin angular momentum:  $\hbar/2$  and  $-\hbar/2$ , and the square of the magnitude of their spin angular momentum is  $s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$ . Also called intrinsic angular momentum or spin.

**spin angular momentum operators**

Quantum-mechanical operators representing the spin

components of a spin- $\frac{1}{2}$  particle, given by the square matrices:

$$\begin{aligned}\hat{S}_x &= \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \hat{S}_y &= \frac{\hbar}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \\ \hat{S}_z &= \frac{\hbar}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.\end{aligned}$$

These matrices satisfy the commutation relations  $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$ ,  $[\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x$  and  $[\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y$ .

The operator representing the spin component of a spin- $\frac{1}{2}$  particle in an arbitrary direction is given by the general spin matrix.

**spin bra vector** A bra vector that represents the spin state of a particle or a system. See also positional convention.

**spin component** A given component of the spin angular momentum, such as  $S_x$  or  $S_y$ . The spin component in the direction of the unit vector  $\mathbf{n} = n_x\mathbf{e}_x + n_y\mathbf{e}_y + n_z\mathbf{e}_z$  is

$$\mathbf{n} \cdot \mathbf{S} = n_x S_x + n_y S_y + n_z S_z.$$

**spin gyromagnetic ratio** (B2: 90) The proportionality constant  $\gamma_s$  that occurs in the equation  $\boldsymbol{\mu} = \gamma_s \mathbf{S}$ , where  $\boldsymbol{\mu}$  is the magnetic dipole moment due to the spin  $\mathbf{S}$ .

**spin ket vector** A ket vector that represents the spin state of a particle or a system. See also positional convention.

**spin magnetic quantum number** (B2: 85) The quantum number  $m_s$  that determines the  $z$ -component of the spin angular momentum of a particle:  $S_z = m_s \hbar$ . For a spin- $\frac{1}{2}$  particle,  $m_s = \pm \frac{1}{2}$ .

**spin precession** (B2: 233) The phenomenon in which the spin components  $S_x$  and  $S_y$  perpendicular to a magnetic field  $\mathbf{B} = B\mathbf{e}_z$  have expectation values that vary sinusoidally in time, and phases that differ by  $\pi/2$ . The angular frequency of the oscillation is equal to the Larmor frequency.

**spin preparer** (B2: 69) A Stern–Gerlach apparatus in which one sub-beam from a beam of spin- $\frac{1}{2}$  particles passes undetected while the other sub-beam is blocked off. All particles leaving the apparatus are in the same spin state. Contrast with spin analyzer.

**spin quantum number** (B2: 85) For a single particle, the spin quantum number is a non-negative integer or half-integer,  $s$ , that determines the square of the magnitude of the spin angular momentum of a particle:

$$S^2 = s(s+1)\hbar^2.$$

For a spin- $\frac{1}{2}$  particle,  $s = \frac{1}{2}$ .

For a *system* of more than one particle, the *total spin quantum number* is generally denoted by  $S$ , and the square of the magnitude of the *total spin angular momentum* of the system is  $S(S + 1)\hbar^2$ . This notation could lead to confusion between the *quantum number*  $S$  and the magnitude of the *vector*  $\mathbf{S}$ , but the meaning is usually clear from context.

**spin space** (B2: 74) A *complex vector space* used to represent the *spin states* of *particles*. For *spin- $\frac{1}{2}$  particles*, spin space is two-dimensional.

**spin state** (B2: 73) A partial specification of the *state* of a *particle* or *system* that refers only to *spin* and omits all spatial information. A spin state is represented by a *spin ket vector* in *spin space*. Compare with *spatial wave function*.

**spin- $\frac{1}{2}$  particle** (B2: 73) A *particle* with *spin quantum number*  $s = \frac{1}{2}$ , and hence a *spin angular momentum* of magnitude  $\sqrt{s(s + 1)}\hbar = (\sqrt{3}/2)\hbar$ , and *spin components* along any axis of  $\pm\hbar/2$ . Examples include *electrons*, *protons*, *neutrons* and *quarks*. Spin- $\frac{1}{2}$  particles are *fermions*, so they have *antisymmetric total wave functions* and obey the *Pauli exclusion principle*.

**spin-down state** (B2: 74) The *spin state* of a *spin- $\frac{1}{2}$  particle* is said to be spin-down relative to a given direction if a *measurement* of the *spin component* in that direction is certain to give the value  $-\hbar/2$ .

**spin-orbit interaction** (B3: 25) An interaction between the *magnetic dipole moments* associated with *spin angular momentum* and *orbital angular momentum*. In a *hydrogen atom*, the spin-orbit interaction is described by a *potential energy function* proportional to  $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}/r^3$ . This adds to the *Hamiltonian operator* for the *Coulomb model* of a hydrogen atom, leading to *fine structure* in hydrogen atom *spectrum*. In the *LS-coupling scheme*, the spin-orbit interaction causes an *atomic term* to split into various *atomic levels* with different *energies*.

**spin-orbit splitting** (B3: 32) The splitting of an otherwise *degenerate energy level* into more than one *energy level* as a result of the *spin-orbit interaction*.

**spin-up state** (B2: 74) The *spin state* of a *spin- $\frac{1}{2}$  particle* is said to be spin-up relative to a given direction if a *measurement* of the *spin component* in that direction is certain to give the value  $+\hbar/2$ .

**spinor** (B2: 77) For a *spin- $\frac{1}{2}$  particle*, a spinor is a two-element *matrix* representing the *spin state* of the particle. The two entries represent the *probability amplitudes* for the particle to be found to have *spin components*  $+\hbar/2$  or  $-\hbar/2$  in the  $z$ -direction.

**spontaneous emission** (B3: 197) A *radiative transition* in which a *system* emits a *photon* and jumps to a *quantum state* of lower *energy* without being induced to do so by external *electromagnetic*

*radiation*. This process conserves energy;  $E_i = E_f + hf$ , where  $E_i$  is the energy of the initial state,  $E_f$  is the energy of the final state and  $hf$  is the energy of the emitted photon.

The rate of spontaneous emission is proportional to the *Einstein A-coefficient*, which can be related to the *Einstein B-coefficient* using the *electric dipole approximation* and *time-dependent perturbation theory*. Vacuum fluctuations are ultimately responsible for provoking a radiative transition between *stationary states*, so fundamental calculations of spontaneous emission require the use of *quantum electrodynamics*. Compare with *stimulated emission* and *absorption*.

**square matrix** (B2: 215) A *matrix* with the same number of rows and columns. An  $n \times n$  square matrix acts as a *linear operator* on an  $n \times 1$  *column matrix*.

**standard deviation** (B1: 116, 230) A quantity that measures the extent by which a set of data values spreads out on either side of the *average value*. The standard deviation of a quantity  $A$  is defined as

$$\sigma(A) = \left[ \overline{(A - \overline{A})^2} \right]^{1/2},$$

where the bars indicate average values. As the number of data values tends to infinity, the standard deviation  $\sigma(A)$  is expected to approach the *uncertainty*  $\Delta A$ .

(Statisticians sometimes use a slightly different quantity called the sample standard deviation. This differs from our definition by an amount that becomes vanishingly small as the number of data values tends to infinity.)

**standing wave** (B1: 73) A *wave* that oscillates without travelling through space. All points in the disturbance that constitutes the wave oscillate *in phase* with the same *frequency* but with different *amplitudes*. The fixed points of zero disturbance are called the *nodes* of the wave (although end-points of the disturbance are not always counted as nodes). A standing wave can be regarded as the sum of two *travelling waves*, propagating in opposite directions.

A familiar example from *classical physics* is the standing wave on a string stretched between fixed endpoints at  $x = 0$  and  $x = L$ . This can be represented by the function

$$u(x, t) = A \sin(kx) \cos(\omega t + \phi),$$

where  $\omega$  is the *angular frequency* and  $k$  is the *wave number*. The possible standing waves are restricted by the requirement that the distance between the fixed ends of the string must be equal to a whole number of half-wavelengths, which implies that  $kL = n\pi$ , where  $n$  is an integer.

In *quantum physics*, a *stationary-state wave function* describes a *complex-valued* standing wave.

**state** (B1: 51) The condition of a *system* described in sufficient detail to distinguish it from other conditions



in which the system would behave differently. In *classical mechanics*, the state of a system of *particles* at a given time can be completely specified by giving the values the positions and velocities of all the particles at that time. In *wave mechanics*, the state of a system at a given time is specified by the *wave function* at that time. Everything that can be said about the *probabilities* of the outcomes of *measurements* is implicit in the wave function.

**BOOK 2:** More generally, the state of a system in *quantum mechanics* is represented by a *state vector*.

**state vector** (B2: 14) An *abstract vector*  $|\Psi\rangle$  that represents the *state* of a *quantum system*.

**state vector collapse** (B2: 86, 136) See *collapse of the state vector*.

**stationary state** (B1: 57) A *quantum state* described by a *wave function* that satisfies *Schrödinger's equation* and is a product of a factor that depends on spatial coordinates and a factor that depends on time. In one dimension, the wave function of a stationary state can be expressed as  $\psi(x)e^{-iEt/\hbar}$ , where  $E$  is the total *energy* of the *system*,  $\psi(x)$  is a solution of the *time-independent Schrödinger equation* corresponding to the *energy eigenvalue*  $E$ , and  $\hbar$  is *Planck's constant* divided by  $2\pi$ .

In any stationary state, the energy has a definite value and the *probability distribution* associated with any *observable* is independent of time.

**Stern–Gerlach apparatus** An apparatus used to carry out *Stern–Gerlach experiments*. The essentials include an oven, a collimator, a vacuum chamber, a *Stern–Gerlach magnet* and particle detectors or beam blockers.

**Stern–Gerlach experiment** (B2: 43) An experiment in which a collimated beam of *atoms* passes through a strongly-inhomogeneous *magnetic field* in a high vacuum. The atoms are deflected by the field and detected after they have left the field. The Stern–Gerlach experiment provides evidence for the *quantization* of *angular momentum*. In the original experiment carried out by Stern and Gerlach, a beam of silver atoms was used; the observation of two emerging sub-beams is evidence for *spin angular momentum*.

**Stern–Gerlach magnet** A magnet used to produce a strongly-inhomogeneous *magnetic field* in a *Stern–Gerlach apparatus*. One pole-piece is pointed and the other notched.

**stimulated emission** (B3: 197) A *radiative transition* in which a *system* is induced by external *electromagnetic radiation* to emit a *photon* and jump to a *quantum state* of lower *energy*. The emitted photon shares the same properties as the photons used to induce the transition (same energy, *polarization*

*state* and direction of motion) and the emitted radiation has the same *wavelength* and *phase* as the incident radiation. The rate of stimulated emission is proportional to the *Einstein B-coefficient*, which can be calculated using the *electric dipole approximation* and *time-dependent perturbation theory*. Compare with *spontaneous emission* and *absorption*.

**STM** An acronym for *scanning tunnelling microscope*.

**superposition principle** (B1: 52) See *principle of superposition*.

**symmetric function** (B2: 110) A function  $f(x_1, x_2)$  is said to be symmetric with respect to exchange of the labels 1 and 2 if

$$f(x_2, x_1) = f(x_1, x_2)$$

More generally, a function of many variables is symmetric if it remains unchanged when any two of its variables are exchanged.

A *triplet spin state* is symmetric and the *spatial wave function* of a pair of *electrons* in a *singlet state* is symmetric. Contrast with *antisymmetric function*.

**symmetric well** (B1: 76) In one dimension, a well described by a *potential energy function*  $V(x)$  with the property  $V(x) = V(-x)$ . Symmetric wells have *energy eigenfunctions* that are either *even functions* or *odd functions*. The even or odd nature of eigenfunctions alternates with increasing *energy*.

**system** The portion of the Universe chosen as the subject of a scientific investigation. See also *isolated system*.

**teleportation** See *quantum teleportation*.

**terms** See *atomic terms*.

**three-dimensional Fourier transform** (B3: 63)

The three-dimensional Fourier transform of a function  $f(\mathbf{r})$  is defined by

$$g(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int f(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}} dV,$$

where the integral is over the whole of space and  $\mathbf{k}$  is called the *wave vector*. The three-dimensional Fourier transform is used to find the *momentum amplitude function* corresponding to a given *wave function* in three dimensions. See also *Fourier transform*.

**three-dimensional infinite square well** (B1: 82) A three-dimensional *potential energy function* that is infinite everywhere except for a finite region, within which the *potential energy* has a constant value (usually taken to be zero). In a three-dimensional infinite square well occupying a cubic region with sides of length  $L$ , with zero potential energy within the well, a *particle* of mass  $m$  has *energy eigenvalues*

$$E_n = \frac{(n_x^2 + n_y^2 + n_z^2)\hbar^2}{2mL^2},$$

where the *quantum numbers*  $n_x$ ,  $n_y$  and  $n_z$  are positive integers. The *energy eigenfunctions* are products of a *sinusoidal* function in  $x$ , a sinusoidal function in  $y$  and a sinusoidal function in  $z$ . Most of these eigenfunctions are *degenerate*.

**tight-binding method** (B3: 180) A method used to find the approximate *energy eigenfunctions* and *eigenvalues* of *electrons* in *crystalline solids*. Each energy eigenfunction is assumed to be of the form

$$\psi_{\mathbf{k}}(\mathbf{r}) = A_{\mathbf{k}} \sum_i e^{i\mathbf{k} \cdot \mathbf{R}_i} \phi(\mathbf{r} - \mathbf{R}_i),$$

where  $\mathbf{k}$  is the *wave vector* that labels the *eigenfunction*,  $A_{\mathbf{k}}$  is a *normalization constant*,  $\mathbf{R}_i$  is a *lattice vector*,  $\phi(\mathbf{r} - \mathbf{R}_i)$  is an *atomic orbital* of a given type centred on  $\mathbf{R}_i$ , and the sum is over all the *lattice points* in the crystal. Such a function is consistent with *Bloch's theorem*. Further approximations are made, including neglecting interactions between the *valence electrons* and ignoring *matrix elements*  $\langle \phi_i | \hat{H} | \phi_j \rangle$  when  $i$  and  $j$  refer to sites further apart than neighbouring sites.

**time-dependent perturbation theory** (B3: 202) A method that gives approximate solutions to *Schrödinger's equation*. The *Hamiltonian operator* of a system is written as the sum of an *unperturbed Hamiltonian*  $\hat{H}^{(0)}$  (with *eigenfunctions*  $\psi_k(x)$  and *eigenvalues*  $E_k$ ) and a *time-dependent perturbation*  $\hat{V}(t)$ . The exact wave function  $\Psi(x, t)$  is then written as a *linear combination* of the unperturbed *stationary-state wave functions*  $\psi_k(x) e^{-iE_k t/\hbar}$ , with time-dependent coefficients  $a_k(t)$ :

$$\Psi(x, t) = \sum_k a_k(t) \psi_k(x) e^{-iE_k t/\hbar}.$$

If the system is initially in the *state*  $i$ , and the perturbation  $\hat{V}(t)$  is switched on at  $t = 0$ , the *first-order approximation* for the coefficient  $a_k(t)$  is

$$a_k(t) \simeq \delta_{ki} + \frac{1}{i\hbar} \int_0^t e^{i\omega_{ki}t'} V_{ki}(t') dt',$$

where  $V_{ki}(t') = \langle \psi_k | \hat{V}(t') | \psi_i \rangle$ .

**time-independent perturbation theory** (B3: 75) A method that gives approximate *energy eigenfunctions* and *energy eigenvalues* for a given system, especially in cases where exact solutions to the *time-independent Schrödinger equation* are difficult or impossible to find. The *perturbation method* is based on expressing the exact *Hamiltonian operator*  $\hat{H}$  for a system as the sum of an *unperturbed Hamiltonian*,  $\hat{H}^{(0)}$  and a relatively small *perturbation*,  $\delta\hat{H}$ :

$$\hat{H} = \hat{H}^{(0)} + \delta\hat{H}.$$

The exact energy eigenfunctions  $\psi_n$  and eigenvalues  $E_n$  are expressed as expansions that involve the

unperturbed energy eigenfunctions  $\psi_n^{(0)}$  and eigenvalues  $E_n^{(0)}$  (which are assumed to be known) and the perturbation,  $\delta\hat{H}$ . Successive terms in the expansions involve increasing powers of the perturbation. The *first-order approximation* for the energy eigenvalue in *quantum state*  $n$  is given by

$$E_n \simeq E_n^{(0)} + \langle \psi_n^{(0)} | \delta\hat{H} | \psi_n^{(0)} \rangle.$$

**time-independent Schrödinger equation** (B1: 55)

An *eigenvalue equation* for *energy*, which can be derived from *Schrödinger's equation* for a system of *particles* with a time-independent *potential energy function*. The time-independent Schrödinger equation can be written in the form

$$\hat{H}\psi = E\psi,$$

where  $\hat{H}$  is the *Hamiltonian operator* of the system,  $\psi$  is an *energy eigenfunction* and  $E$  is the corresponding *energy eigenvalue*.

For a one-dimensional system consisting of a particle with potential energy function  $V(x)$ , the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x),$$

where  $\hbar$  is *Planck's constant* divided by  $2\pi$ .

BOOK 2: In *Dirac notation*, the time-independent Schrödinger equation is

$$\hat{H}|\psi\rangle = E|\psi\rangle.$$

This equation also applies to the *spin states* of a *spin- $\frac{1}{2}$  particle*, with  $|\psi\rangle$  represented by a *column spinor* and  $\hat{H}$  by a  $2 \times 2$  *square matrix*.

**total angular momentum** (B3: 26) The sum of the *orbital angular momentum*  $\mathbf{L}$  and the *spin angular momentum*  $\mathbf{S}$  of a given system:

$$\mathbf{J} = \mathbf{L} + \mathbf{S}.$$

In *Cartesian coordinates*,  $J_z = L_z + S_z$  (with similar results for the  $x$  and  $y$ -components) and  $J^2 = J_x^2 + J_y^2 + J_z^2$ . The corresponding quantum-mechanical operators are  $\hat{J}_z$  and  $\hat{J}^2$ .

For a single particle, the *eigenvalues* of  $J^2$  are  $j(j+1)\hbar^2$ , where  $j$  is *total angular momentum quantum number* of the particle, and the eigenvalues of  $J_z$  are  $m_j$ , where  $m_j = -j, -j+1, \dots, j-1, j$  is the *total magnetic quantum number* of the particle.

For a system, the total angular momentum quantum number is written as  $J$ , and the total magnetic quantum number is written as  $M_J$ . The eigenvalues of  $J^2$  and  $J_z$  are then  $J(J+1)\hbar^2$ , and  $J_z$  are  $M_J\hbar$  respectively.

In the presence of a *spin-orbit interaction*, a *spin- $\frac{1}{2}$  particle* in a *spherically-symmetric potential energy well*, or an *atom* in the *central-field approximation* have operators  $\hat{J}^2$  and  $\hat{J}_z$  that *commute* with one

another and with the *Hamiltonian operator* of the system. The eigenvalues of these operators are *good quantum numbers* that can be used to label the *stationary states* of the system. See also *atomic levels*.

### total angular momentum operators

Quantum-mechanical *operators* representing the *components* of the *total angular momentum*  $\mathbf{J}$  of a system. For a system with *orbital angular momentum*  $\mathbf{L}$  and *spin angular momentum*  $\mathbf{S}$ , the total angular momentum operators are

$$\hat{J}_x = \hat{L}_x + \hat{S}_x$$

$$\hat{J}_y = \hat{L}_y + \hat{S}_y$$

$$\hat{J}_z = \hat{L}_z + \hat{S}_z,$$

where the *orbital angular momentum operators*  $\hat{L}_x$ ,  $\hat{L}_y$  and  $\hat{L}_z$  act only of spatial parts of the *total wave function*, and the *spin angular momentum operators*  $\hat{S}_x$ ,  $\hat{S}_y$  and  $\hat{S}_z$  act only on spin parts.

Total angular momentum operators satisfy the *commutation relations*  $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$ ,  $[\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x$  and  $[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$ .

### total angular momentum quantum number

(B3: 28) The *quantum number* that determines the possible values of the *total angular momentum* of a *particle* or *system*.

For a *spin- $\frac{1}{2}$  particle*, the total angular momentum quantum number is written as  $j$  and the *eigenvalues* of  $\hat{J}^2$  are  $j(j+1)\hbar^2$ . In this case,

$$j = \begin{cases} \frac{1}{2} & \text{if } l = 0 \\ l \pm \frac{1}{2} & \text{if } l \neq 0, \end{cases}$$

where  $l$  is the *orbital angular momentum quantum number*.

For an *atom* in the *LS-coupling scheme*, the total angular momentum quantum number is written as  $J$  and the eigenvalues of  $\hat{J}^2$  are  $J(J+1)\hbar^2$ . In this case, the allowed values of  $J$  are

$$|L - S|, |L - S| + 1, \dots, |L + S| - 1, |L + S|$$

where  $L$  is the *total orbital angular momentum quantum number* of the atom and  $S$  is the *total spin quantum number*.

### total atomic angular momentum (B3: 136)

The *total angular momentum* of an *atom*, well-approximated by adding together the *orbital angular momenta* and the *spin angular momenta* of all the *electrons* in the atom, using the *LS-coupling scheme* for atoms of low *atomic number* and the *jj-coupling scheme* for atoms of high atomic number.

**total cross-section** (B1: 196) A quantity used to measure the total rate per unit time per unit incident

*flux*, at which a given type of target scatters a given type of incident *particle*. The *SI* unit of total cross-section is  $\text{m}^2$  but the *barn* is a more commonly-used unit in particle and nuclear physics.

**total magnetic quantum number** (B3: 28) The *quantum number* that determines the *eigenvalues* of  $\hat{J}_z$ , the *operator* for the  $z$ -component of the *total angular momentum*.

For a *particle*, the total magnetic quantum number is written as  $m_j$  and the eigenvalues of  $\hat{J}_z$  are  $m_j\hbar$ . In this case, the allowed values of  $m_j$  are  $-j, -j+1, \dots, j-1, j$ , where  $j$  is the *total angular momentum quantum number*.

For a *system*, the total magnetic quantum number is written as  $M_J$  and the eigenvalues of  $\hat{J}_z$  are  $M_J\hbar$ . In this case, the allowed values of  $M_J$  are  $-J, -J+1, \dots, J-1, J$ , where  $J$  is the total angular momentum quantum number.

**total orbital angular momentum** The *vector sum* of the *orbital angular momenta* of all the *particles* in a given system. Used in the *LS-coupling scheme*.

### total orbital angular momentum quantum number

(B3: 134) The *quantum number*,  $L$ , such that the possible values of the square of the *magnitude* of the *total orbital angular momentum* are  $L(L+1)\hbar^2$ .

For a two-particle system composed of particle 1 with *orbital angular momentum quantum number*  $l_1$ , and particle 2 with *orbital angular momentum quantum number*  $l_2$ , the possible values of  $L$  are

$$|l_1 - l_2|, |l_1 - l_2| + 1, \dots, |l_1 + l_2| - 1, |l_1 + l_2|.$$

**total spin angular momentum** The *vector sum* of the *spin angular momenta* of all the *particles* in a system. Used in the *LS-coupling scheme*.

**total spin quantum number** (B3: 134) A *quantum number*,  $S$ , such that the possible values of the square of the *magnitude* of the *total spin angular momentum* are  $S(S+1)\hbar^2$ .

For a two-particle system composed of particle 1 with *spin quantum number*  $s_1$ , and particle 2 with *spin quantum number*  $s_2$ , the possible values of  $S$  are

$$s_1 - s_2, |s_1 - s_2| + 1, \dots, |s_1 + s_2| - 1, |s_1 + s_2|.$$

For two *spin- $\frac{1}{2}$  particles*,  $S = 0$  or  $S = 1$ .

**total static energy** (B3: 145) The *electronic energy* of a *molecule* plus the *electrostatic potential energy* due to the mutual repulsion of its *nuclei*. In the *Born–Oppenheimer approximation*, this provides an *effective potential energy function* in which the nuclei move. The total static energy is not the same as the total *energy* of the molecule, which includes the rotational and vibrational energies associated with nuclear motion.

**total wave function** (B2: 105) A description of a *system* that specifies both the *spatial wave function*



and the *spin ket vector* of the system. Any system of *identical bosons* has a *symmetric* total wave function. Any system of *identical fermions* has an *antisymmetric* total wave function.

**transition probability** (B3: 207) The *probability*  $P_{i \rightarrow f}(t)$  that a *system*, initially in the *state*  $i$  at  $t = 0$ , will be found in some other *state*  $f$  at a later time  $t$ .

**translational symmetry** (B3: 170) A *system* is said to have translational symmetry if its properties do not change when it is viewed from a different point in space. An infinite *crystal* has translational symmetry with respect to displacements by its *lattice vectors*.

**transmission coefficient** (B1: 182) The *probability* that a specified one-dimensional *potential energy function* will allow an incident *particle* to pass through, continuing in its original direction of motion. Compare with *reflection coefficient*.

**transmission resonance** (B1: 194) For one-dimensional *scattering*, a transmission resonance is a maximum in the *transmission coefficient*  $T$  as a function of *energy*, ideally with  $T = 1$ , corresponding to perfect transmission and no reflection.

**transverse wave** A *wave* composed of *oscillations* that take place in a direction perpendicular to the direction of propagation of the wave. Contrast with *longitudinal wave*.

**travelling wave** A *wave* that propagates from one place to another. A one-dimensional example of such a wave is represented by the function

$$u(x, t) = A \cos(kx - \omega t + \phi),$$

where the positive constant  $A$  is the *amplitude*,  $k$  is the *wave number*,  $\omega$  is the *angular frequency* and  $\phi$  is the *phase constant*. The quantity  $kx - \omega t + \phi$  is the *phase* of the wave. Contrast with *standing wave*.

**trial function** (B3: 68) In the *variational method*, the trial function is an educated guess made for an *energy eigenfunction* of a given *system*. The trial function  $\psi$  may contain one or more adjustable parameters, and an approximation for the *energy eigenvalue* is provided by a stationary value of  $\langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$ , where  $\hat{H}$  is the *Hamiltonian operator* of the system. In the case of the *ground state*, the minimum possible value of  $\langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$  gives an estimate that is always greater than or equal to the ground-state *energy*.

**triangle inequality** (B2: 206) For two *ordinary vectors*  $\mathbf{a}$  and  $\mathbf{b}$ , the triangle inequality states that

$$|\mathbf{a} + \mathbf{b}| \leq |\mathbf{a}| + |\mathbf{b}|.$$

**triangle rule** (B2: 206) A geometric rule for adding two *ordinary vectors*. Arrows representing the vectors are drawn with the head of the first arrow,  $\mathbf{a}$ , coincident with the tail of the second arrow,  $\mathbf{b}$ . The

arrow joining the tail of  $\mathbf{a}$  to the head of  $\mathbf{b}$  then represents the vector sum  $\mathbf{a} + \mathbf{b}$ .

**triple bond** (B3: 164) In the *LCAO approximation* for *molecules*, a chemical bond with a *formal bond order* of 3 is referred to as a triple bond.

**triplet state** (B2: 113) A *spin state* of a *system* of two *spin- $\frac{1}{2}$  particles* for which the *total spin quantum number* is  $S = 1$ . There are three such spin states, with *spin magnetic quantum numbers*  $M_S = 1, 0$  and  $-1$ . Each of these states is *symmetric* with respect to exchange of the particle labels and is accompanied by an *antisymmetric spatial wave function*. Compare with *singlet state*.

**tunnelling** (B1: 179) The quantum-mechanical phenomenon in which an incident *particle*, initially in a classically-allowed region, is able to pass through a *classically-forbidden region* and emerge on the far side of it, travelling in another classically-allowed region. Such tunnelling cannot occur in *classical physics* because the particle is unable to enter the classically-forbidden region, where the particle's total *energy* is less than its *potential energy*.

Tunnelling occurs in *alpha decay*, *nuclear fusion* in the *proton-proton chain* and the *scanning tunnelling microscope*.

**twenty-one centimetre radiation** (B3: 108) *Electromagnetic radiation* of wavelength 21 cm emitted by *hydrogen atoms* making a *radiative transition* between the two *hyperfine atomic levels* of the *ground-state electronic configuration*. The two hyperfine levels have  $F = 1$  and  $F = 0$ , where  $F$  is the *total spin quantum number* associated with the combined spins of the *electron* and the *proton*. This radiation is detected by astronomers investigating the distribution and motion of relatively cold hydrogen atoms in the Universe.

**two-dimensional infinite square well** (B1: 78) A two-dimensional *potential energy function* that is infinite everywhere except for a finite region, within which the *potential energy* has a constant value (usually taken to be zero). In a two-dimensional infinite square well occupying a square region with sides of length  $L$ , with zero potential energy within the well, a *particle* of mass  $m$  has *energy eigenvalues*

$$E_n = \frac{(n_x^2 + n_y^2)\hbar^2}{2mL^2},$$

where the *quantum numbers*  $n_x$  and  $n_y$  are positive integers. The *energy eigenfunctions* are products of a *sinusoidal function* in  $x$  and a *sinusoidal function* in  $y$ . Most of these eigenfunctions are *degenerate*.

**two-slit interference pattern** (B1: 18) The pattern of *interference maxima* and *interference minima* that forms when a *plane wave* is incident on an absorbing screen containing two narrow slits. The pattern,

formed on the far side of the absorbing screen, consists of a series of bright bands separated by dark bands. The bright bands occur in places where the waves passing through the two slits interfere constructively. The dark bands occur in places where these waves interfere destructively. The two slits must be narrow enough for their two *diffraction patterns* to appreciably overlap. This implies that their widths must be comparable to, or smaller than, the *wavelength* of the incident wave. See also *constructive interference* and *destructive interference*.

**uncertainty** (B1: 116, 231) The quantum-mechanical prediction for the *standard deviation* of an *observable* in a *system* in a given *state*. The uncertainty is defined by

$$\Delta A = [\langle (A - \langle A \rangle)^2 \rangle]^{1/2}$$

where angular brackets denote *expectation values* and  $(A - \langle A \rangle)^2$  is the square of the deviation of  $A$  from its expectation value. Uncertainties can also be calculated from the formula

$$\Delta A = [\langle A^2 \rangle - \langle A \rangle^2]^{1/2}.$$

**uncertainty principle** A shorthand term for the *Heisenberg uncertainty principle* or the *generalized uncertainty principle*.

**ungerade orbital** (B3: 158) A *molecular orbital* in a *diatomic molecule* that has *odd parity* under the operation of *inversion* about the *centre of symmetry* of the molecule. The word ‘ungerade’ means ‘odd’ in German. Ungerade orbitals are indicated by the subscript u. Contrast with *gerade*.

**unit matrix** (B2: 217) A *matrix* with 1’s along its main diagonal and zeros elsewhere. Any  $n \times n$  *square matrix* is unchanged when multiplied by an  $n \times n$  unit matrix.

**unit vector** (B2: 205) A *vector* of unit *magnitude* in a given direction. A unit vector is dimensionless (it has no units).

**unperturbed Hamiltonian** (B3: 76) A *Hamiltonian* whose *eigenfunctions* and *eigenvalues* are known and which provides an approximation to a more complicated Hamiltonian whose eigenfunctions or eigenvalues we wish to approximate.

**valence band** (B3: 189) In a *semiconductor* or *insulator*, the valence band is the highest *energy band* that is fully occupied at *absolute zero*. At non-zero temperatures, the valence band of a semiconductor is occupied by a small number of *holes* as a result of thermal excitation of *electrons* from the valence band to the *conduction band* or to *acceptor atom states* just above the valence band. Contrast with *conduction band*.

**valence electron** (B3: 127) An *electron* in an *open shell* of an *atom*. The valence electrons in an atom determine many of its properties.

**variational method** (B3: 67) A method used to estimate the *energy* of the *ground state* of a *quantum system*. The method is based on guessing a *trial function* that should be similar to the ground-state *eigenfunction* of the *Hamiltonian operator*  $\hat{H}$  of the system. The trial function generally includes one or more adjustable parameters, and the quantity  $\langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$  is minimized with respect to these adjustable parameters. The minimum value is the best estimate of the ground-state energy for the chosen trial function, and is always greater than or equal to the true ground-state energy.

Under favourable circumstances, the method can be extended to give estimates of *excited-state energy eigenvalues*. This is done by choosing an appropriate trial function  $\psi$  and adjusting it to give a stationary value of  $\langle \psi | \hat{H} | \psi \rangle / \langle \psi | \psi \rangle$ .

**vector** (B2: 205, 212) (i) A quantity with a definite *magnitude* and a definite direction in space, also called an ordinary vector. Ordinary vectors can be specified by giving their *components* in a three-dimensional coordinate system.

(ii) More generally, *abstract vectors* in a *vector space* are entities (denoted by  $|a\rangle$ ,  $|b\rangle$ ,  $|c\rangle$ , ...) that obey the following rules:

1. Any two vectors can be added, and the result is a vector; this operation obeys the rules:

$$|a\rangle + |b\rangle = |b\rangle + |a\rangle$$

$$(|a\rangle + |b\rangle) + |c\rangle = |a\rangle + (|b\rangle + |c\rangle).$$

2. There is a *zero vector*, denoted by  $|0\rangle$ , such that

$$|a\rangle + |0\rangle = |a\rangle \quad \text{for any vector } |a\rangle.$$

3. Any vector can be multiplied by a *scalar*, and the result is a vector; this operation obeys the rules:

$$\alpha(\beta|a\rangle) = (\alpha\beta)|a\rangle$$

$$(\alpha + \beta)|a\rangle = \alpha|a\rangle + \beta|a\rangle$$

$$\alpha(|a\rangle + |b\rangle) = \alpha|a\rangle + \alpha|b\rangle.$$

4. Multiplication of any vector  $|a\rangle$  by 0 and 1 give

$$0|a\rangle = |0\rangle$$

$$1|a\rangle = |a\rangle.$$

**vector product** (B2: 209) The vector product of two *vectors* **a** and **b** is a vector quantity defined by

$$\mathbf{a} \times \mathbf{b} = (a_y b_z - a_z b_y) \mathbf{e}_x + (a_z b_x - a_x b_z) \mathbf{e}_y + (a_x b_y - a_y b_x) \mathbf{e}_z,$$

where the *components* of the vectors are taken in a right-handed *Cartesian coordinate system* with

**unit vectors**  $\mathbf{e}_x$ ,  $\mathbf{e}_y$  and  $\mathbf{e}_z$ . The vector product has *magnitude*  $ab \sin \theta$ , where  $\theta$  is the angle between the directions of the vectors taken to be in the range  $0 \leq \theta \leq \pi$ . Its direction is given by the *right-hand rule*.

**vector space** (B2: 13, 212) A set of *vectors* generated by exhaustively applying the operations of vector addition and *scalar* multiplication to a given set of vectors.

**vertical polarization** Given a fixed axis perpendicular to the direction of propagation of *linearly-polarized* light, the *light* is said to be vertically polarized relative to the given axis if its *electric field* is always parallel or antiparallel to the axis. Contrast with *horizontal polarization*.

**visible light** *Electromagnetic radiation* with *wavelength* between about  $4 \times 10^{-7}$  m (400 nm, violet) and  $7 \times 10^{-7}$  m (700 nm, red), or equivalently with *frequency* between about  $8 \times 10^{14}$  Hz and  $4 \times 10^{14}$  Hz.

**watt** The *SI* unit of power, or of the rate at which *energy* is transferred, represented by the symbol W. One watt is defined by  $1 \text{ W} = 1 \text{ J s}^{-1}$ .

**wave** A periodic disturbance that travels from one point to another. If the wave travels through a material medium, no *particle* in the medium is permanently displaced by passage of the wave. Waves may be *standing* or *travelling*. Some waves may be *transverse* or *longitudinal*. Transverse waves may be characterized by their polarization. Waves may also be characterized by their *frequency*, *wavelength* and direction of propagation.

**wave function** (B1: 24, 49) A function that fully describes the *quantum state* of a *system* in *wave mechanics*. For a single *particle* in one dimension, the wave function takes the form  $\Psi(x, t)$ . The wave function evolves in time according to *Schrödinger's equation*, except when the system is disturbed by a *measurement*, leading to the *collapse of the wave function*.

The spatial extent of a particle's wave function is not to be confused with the size of the particle. For example, the spatial extent of the wave function of an *electron* in a *hydrogen atom* is the spatial extent of the atom, whilst the electron itself is much smaller, a point particle as far as we can tell.

**wave mechanics** (B1: 7) A term given to a way of formulating *quantum mechanics*, and carrying out quantum-mechanical calculations, pioneered by Erwin Schrödinger. In wave mechanics, the *state* of a *system* is described by a *wave function*, which obeys a *partial differential equation* called *Schrödinger's equation*. *Observable* quantities are represented by *linear differential operators* that act on the wave function.

**wave number** (B1: 17) A quantity  $k = 2\pi/\lambda$

that describes a *monochromatic wave*, where  $\lambda$  is the *wavelength* of the wave. Wave numbers label *momentum eigenfunctions* in one dimension.

**wave packet** (B1: 150) A *wave function* that is a discrete or continuous *linear combination* of two or more different *stationary-state* wave functions. Any wave function (other than one describing a stationary state) can normally be expressed in this way.

**wave vector** (B3: 176) For a *plane wave* in three dimensions, the wave vector is a *vector* that points in the direction of propagation of the wave, with *magnitude* equal to the *wave number*  $k = 2\pi/\lambda$ , where  $\lambda$  is the *wavelength* of the wave. Wave vectors label *momentum eigenfunctions* in three dimensions. They also label *Bloch wave energy eigenfunctions* in a *crystal*.

**wave-packet spreading** (B1: 172) The phenomenon whereby a *particle* described by a *wave packet* has an *uncertainty* in position that changes (normally increases) with time.

**wave-particle duality** (B1: 17) The phenomenon whereby *systems* display properties associated with both *particles* and *waves* according to the kind of *measurements* performed on them. It shows that it is best to think of 'particle' and 'wave' as categories associated with our macroscopic world; there is no obligation for microscopic entities to fall wholly into one category or the other.

**wavelength** (B1: 17) The spatial separation  $\lambda$ , measured along the direction of propagation, of successive points in a *wave* that differ in *phase* by  $2\pi$  at any fixed time  $t$ . More crudely, the distance between successive peaks of the wave.

**Wollaston prism** A type of *polarizing beam splitter* constructed from a *birefringent material* by cementing together two right-angled triangular prisms of the material, with perpendicular anisotropy axes.

**X-rays** *Electromagnetic radiation* with *wavelength* between  $1 \times 10^{-8}$  m and  $1 \times 10^{-11}$  m, or equivalently *frequency* between about  $3 \times 10^{16}$  Hz and  $3 \times 10^{19}$  Hz.

**zero of potential energy** A point at which the *potential energy* of a *particle* is set equal to zero.

**zero vector** (B2: 16, 206) A *vector* that can be added to any other vector and leave that vector unchanged. The zero vector has zero *norm* and all its *components* are zero. In *function space*, the zero vector corresponds to a function with a vanishing *normalization integral*.

**zero-point energy** (B1: 130) The *ground-state energy* of a *particle*, measured from the bottom of its *potential energy* well. This energy is present even at the *absolute zero* of temperature.

**zeroth-order approximation** (B3: 80) See *order of approximation*.







